JuanB Perez/DC/USEPA/US
11/29/2006 08:23 AM

To NCIC HPV@EPA
cc
bcc
Subject Fw: Email #1 - sec Butyl Ether (CAS #6863-58-7) HPV Program Submission - ExxonMobil Chemical Co

----- Forwarded by JuanB Perez/DC/USEPA/US on 11/29/2006 08:23 AM -----

douglas.a.winkelmann@exxonmobil.com
11/28/2006 12:27 PM

To NCIC OPPT@EPA, Rtk Chem@EPA
cc nigel.j.sarginson@exxonmobil.com
Subject Email #1 - sec Butyl Ether (CAS #6863-58-7) HPV Program Submission - ExxonMobil Chemical Co

Re: HPV Challenge Program - Submission of ExxonMobil Chemical Company Test Plan and Dossier for sec Butyl Ether (CAS #6863-58-7) under the HPV Challenge Program (ExxonMobil Chemical Company Registration Number _____ for HPV Challenge Program)

This submission is contained in two separate emails. The attachments to this first email include:

- sec Butyl Ether HPV - EPA Submission Letter 28Nov06
- sec Butyl Ether 6863-58-7 HPV Test Plan 28Nov06
- 6863-58-7 sBE HPV Dossier 14Nov06
- 108-20-3 DIPE HPV Dossier 27Feb06

The attachments to the second email include:

- 78-92-2 sBA HPV Dossier 01Jun06
- 6863-58-7 sBE HPV Dossier 14Nov06 Export File
- 108-20-3 DIPE HPV Dossier 27Feb06 Export File
- 78-92-2 sBA HPV Dossier 01Jun06 Export File

If you have any questions on the contents of either email, please contact Douglas Winkelmann (contact information follows below).

Regards,
Douglas Winkelmann

ExxonMobil Biomedical Sciences, Inc.
douglas.a.winkelmann@exxonmobil.com
Ph 908.730.1007

(See attached file: sec Butyl Ether HPV - EPA Submission Letter 28Nov06.doc)

(See attached file: sec Butyl Ether 6863-58-7 HPV Test Plan 28Nov06.doc)

(See attached file: 6863-58-7 sBE HPV Dossier 14Nov06.rtf)

(See attached file: 108-20-3 DIPE HPV Dossier 27Feb06.rtf)


sec Butyl Ether HPV - EPA Submission Letter 28Nov06.doc


sec Butyl Ether 6863-58-7 HPV Test Plan 28Nov06.doc


6863-58-7 sBE HPV Dossier 14Nov06.rtf


108-20-3 DIPE HPV Dossier 27Feb06.rtf

Via Electronic Submission

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Nigel J. Sarginson
Manager
Product Stewardship & Regulatory Affairs
Intermediates Americas

ExxonMobil Chemical

November 28, 2006

Stephen L. Johnson
Administrator
U.S. Environmental Protection Agency
P. O. Box 1473
Merrifield, VA 22116

Re: HPV Challenge Program - Submission of ExxonMobil Chemical Company Test Plan and Dossier for sec Butyl Ether (CAS #6863-58-7) under the HPV Challenge Program (ExxonMobil Chemical Company Registration Number _____ for HPV Challenge Program)

Dear Mr. Johnson:

ExxonMobil Chemical Company (EMCC) is strongly committed to the chemical industry's Responsible Care® program and takes seriously its commitment to the responsible manufacture, testing, and safe use of its products. As further evidence of this commitment, EMCC agreed to develop study summaries and hazard testing plans for over 130 chemicals under the U.S. Environmental Protection Agency (EPA) and International Council of Chemical Associations' High Production Volume (HPV) programs.

By copy of this letter, EMCC reaffirms its commitment to providing select data that can be used to characterize the hazard of sec-butyl ether (sBE; CAS #6863-58-7) under the HPV Program. Enclosed is the test plan and dossier for sBE, together with dossiers for diisopropyl ether (CAS #108-20-3) and sec-butyl alcohol (CAS #78-92-2). Following a review of the data for sBE, analogs, and potential metabolites, it was determined that sufficient data are available to characterize all endpoints under the U.S. EPA HPV Program.

Please contact me if you require any further information on the status of EMCC commitments to the U.S. HPV Program.

Sincerely,

Nigel J. Sarginson
ExxonMobil Chemical Company
Product Stewardship & Regulatory Affairs Manager
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Houston, TX 77079

Email: nigel.j.sarginson@exxonmobil.com

Attachment

Cc:

Mr. Charles M. Auer
Director
Office of Pollution Prevention and Toxics (OPPT)
U.S. Environmental Protection Agency (EPA)
1200 Pennsylvania Ave., NW
Washington, DC 20460-0001

HIGH PRODUCTION VOLUME (HPV)

CHEMICAL CHALLENGE PROGRAM

TEST PLAN

For

sec-Butyl Ether

CAS No. 6863-58-7

Prepared by:

ExxonMobil Chemical Company

November 28, 2006

EXECUTIVE SUMMARY

Under the U.S. Environmental Protection Agency (EPA) High Production Volume (HPV) Chemical Challenge Program (Program), ExxonMobil Chemical Company committed to voluntarily compile data that can be used in an initial assessment to characterize the hazard of sec-butyl ether (sBE; CAS No. 6863-58-7). The data for this assessment include selected physicochemical, environmental fate, and human and environmental toxicity endpoints identified by the U.S. HPV Program.

A search for studies and their review identified limited data for sBE to characterize the mammalian and environmental toxicity endpoints for the HPV Program. However, the mammalian endpoints can be characterized with data for sec-butyl alcohol (sBA; 2-butanol) and methyl ethyl ketone (MEK; 2-butanone) which are metabolites of sBE, while the environmental endpoints can be characterized with data for an analog ether and calculated toxicity data.

Results of Mackay Level I distribution modeling show, at steady state, that sBE will partition primarily to the air compartment (99.1%), with a negligible amount partitioning to water (0.5%) and soil (0.4%). Level III modeling indicates, at steady state, that water and soil are the primary compartments on a percentage basis when the default emission to each of these compartments is included in the calculations. However, Level III modeling may not be representative of the ultimate disposition of sBE because default emissions, which use 1000 kg/h/compartment, are not representative of chemical discharge.

sBE is volatile, and in the atmosphere it can be quickly degraded by indirect photolysis. The sBE half-life from hydroxyl radical attack is calculated as approximately 4 hours. Aqueous photolysis and hydrolysis will not contribute to the transformation of sBE in aquatic environments because it is either poorly or not susceptible to these reactions.

sBE has a potential to biodegrade slowly based on results of biodegradation modeling. However, a number of published studies in which non-standard guideline methods were used have demonstrated that alkyl ethers can be degraded by pure strains and mixed cultures of bacteria when incubated under aerobic conditions. The rate of biodegradation for these substances, however, is slow. Despite its potential to biodegrade at a slow rate, sBE is not expected to bioaccumulate, based on a low bioconcentration factor (BCF = 32).

Results of Quantitative Structure Activity Relationship (QSAR) modeling suggest that sBE will exhibit moderate aquatic toxicity. Estimates include a 96-hour LC_{50} value of 14.7 mg/l for a freshwater fish; a 48-hour EC_{50} value of 16.7 mg/l for a freshwater invertebrate; and a 96-hour EC_{50} value of 11.0 mg/l for a green alga. Experimental results for an analog substance, n-butyl ether (nBE), support the use of the modeled data to assess the aquatic hazard of sBE. The 48-hour LC_{50} value for nBE was 30.7 mg/l.

Based on data for sBA and MEK, the degradation products of sBE, sBE is expected to present a low order of hazard for human health. sBE presents a moderate order of hazard for environmental health. In the environment, sBE is calculated to partition primarily to the soil, water, and air phases, where biological and physical processes

mediate its degradation. Given the available data for sBE and its metabolites, no additional testing is proposed.

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sec-Butyl Ether

I. INTRODUCTION

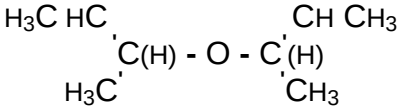
Under the U.S. Environmental Protection Agency (EPA) High Production Volume (HPV) Chemical Challenge Program (Program), ExxonMobil Chemical Company committed to voluntarily compile data that can be used in an initial assessment to characterize the hazard of sec-butyl ether (sBE; CAS No. 6863-58-7). This substance is supported by selected screening data needed for an initial assessment of physicochemical properties, environmental fate, and human and environmental effects endpoints identified by the U.S. HPV Program.

Procedures to assess the reliability of selected data for inclusion in this test plan were based on guidelines described by Klimisch *et al*. (1997) and identified within the U.S. EPA (1999a) document titled Determining the Adequacy of Existing Data.

II. CHEMICAL DESCRIPTION

sBE is a small molecular weight ether represented by the following chemical formula and structures:

$C_8H_{18}O$ $(CH_3\ CH)(CH_3)CHOCH(CH_3)(CH\ CH_3)$



III. TEST PLAN RATIONALE

Data used to characterize the physicochemical, mammalian and environmental toxicity, and environmental fate endpoints in the HPV Program are described below.

A literature and company search for mammalian and environmental toxicity data for sBE did not identify measured data. However, analog and metabolite data were identified that can be used to characterize the hazard of sBE for the mammalian endpoints, while adequate calculated data were developed to characterize the acute and chronic aquatic toxicity of sBE.

This assessment considered that mammalian exposure to sBE would result in potential exposures to 2-butanol (sec-butyl alcohol or sBA; CAS No. 78-92-2) and 2-butanone (methyl ethyl ketone or MEK; CAS No. 78-93-3) as metabolites of sBE. sBE has the potential to hydrolyze, resulting in two molecules of sBA. In mammalian systems sBA is either conjugated and excreted, or fairly rapidly metabolized by alcohol dehydrogenase to MEK. MEK is further metabolized to 3-hydroxy-2-butanone and 2,3-butanediol, which can also be conjugated and excreted. Data from the analog, diisopropyl ether (DIPE; CAS No. 108-20-3), are also provided as read-across data to characterize the toxicity of the parent molecule, sBE.

Data to characterize the aquatic toxicity endpoints were developed using the ECOSAR computer model (ECOSAR, 2004) provided within EPI Suite™ (2000). This model applies an equation for neutral organics to estimate aquatic toxicity and is therefore considered appropriate to estimate aquatic toxicity for sBE. As further justification, calculated data from this model for the fish effect endpoint is consistent with measured

data for an analog ether, supporting the model's use to provide adequate aquatic toxicity data for sBE.

A. Physicochemical Data

Physicochemical data (Table 1) include both calculated and measured data provided by the EPI Suite™ model (EPI Suite, 2000), as discussed in the EPA document titled The Use of Structure-Activity Relationships (SAR) in the High Production Volume Chemicals Challenge Program (US EPA, 1999b). The measured values were supplied by the database of experimental values contained within the EPI Suite model.

Table 1. Selected Physicochemical Properties for sBE.

Data Source	Melting Point (ºC)	Boiling Point (ºC)	Vapor Pressure (hPa @ 25ºC)	Water Solubility (mg/L@ 25ºC)	Log K_{ow} (25ºC)
Calculated	-73	116	29.7	327	2.87
Measured	-100*	na	21.7*	330**	3.35**

* Measured value for sBE from the experimental values database contained within EPI Suite
** Measured value for the analog n-butyl ether
na Data not available for this endpoint

B. Mammalian Toxicity Data

Metabolite and Analog Justification

As discussed in the Test Plan Rationale, data are available for sBA on the following endpoints: acute toxicity (oral, inhalation, dermal), irritation (skin, eye, respiratory tract), reproductive toxicity, developmental toxicity, and genotoxicity. MEK is a major metabolite of sBA and based on its structural similarity with sBA, it's data will be used to address the repeated dose toxicity and supplement the genotoxicity endpoints for sBE. Additionally, diisopropyl ether (DIPE) is a small molecular weight ether similar to sBE and the mammalian toxicity data identified for DIPE can be used as an analog to characterize the mammalian toxicity of sBE, as their inherent toxicities are expected to be similar.

Toxicokinetics and Metabolism

There are several animal studies indicating that sBA is readily absorbed, metabolized to MEK and other subsequent metabolites, and excreted.

Saito (1975) administered 2 ml/kg sBA (approximately 1.6 g/kg) orally to rabbits and blood samples were collected and analyzed by gas chromatography. Approximately 1 mg/ml sBA was found in blood after 1 hour, with 0.7 mg/ml present after 7 hours, and only trace amounts after 10 hours. sBA was metabolized via alcohol dehydrogenase to MEK, which was detected in the blood, reaching its maximum level in the blood after 6 hours. sBA was excreted via exhalation (3.3% of the original dose) and urine (2.6%), but more of the original sBA was excreted as its metabolite MEK. MEK excretion via exhalation and urine were 22.3% and 4.1% of the original dose, respectively. In another

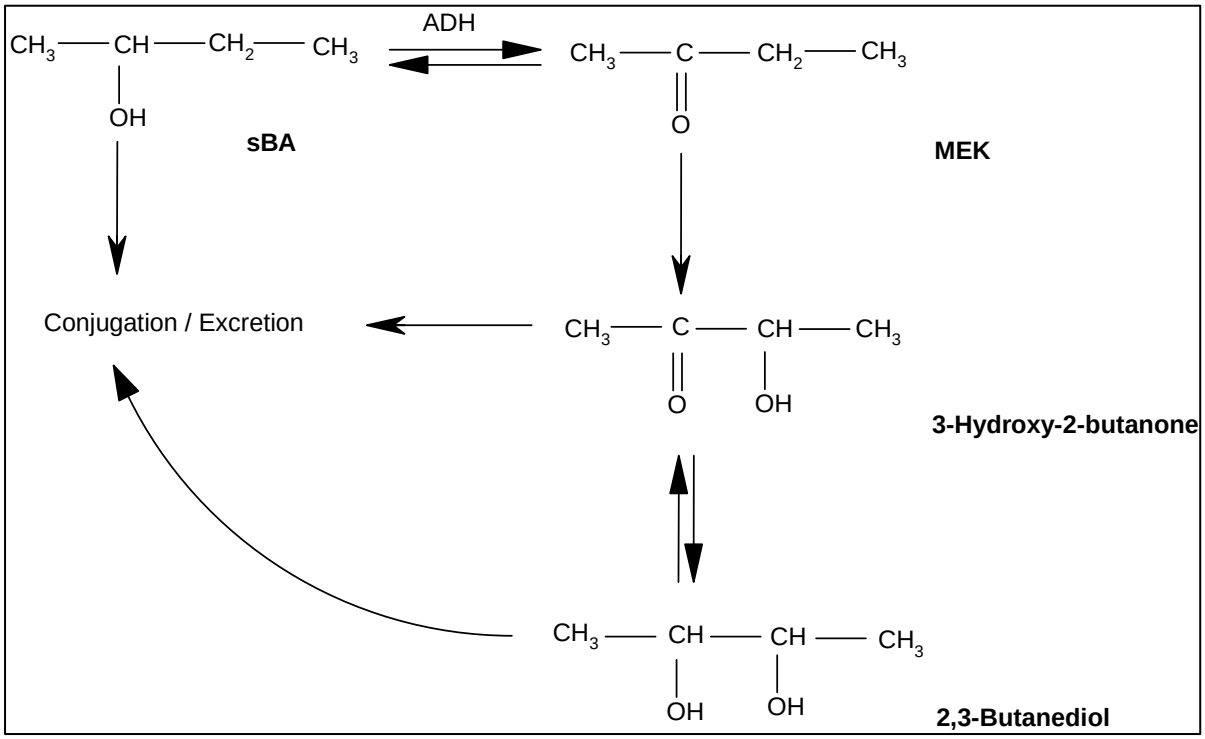
study, 14% of an 8 mmol/kg [approximately 600 mg/kg] oral dose of sBA in rabbits was excreted in the urine as a glucuronic acid conjugate (Kamil, 1952 as cited by Williams, 1959). Majority of the remaining dose was metabolized to MEK.

In rats, Traiger and Bruckner (1976) found a blood elimination half-life of 2.5 hours (after an oral dose of 2.2 ml/kg). One hour after administration, a maximum blood sBA level of 800 mg/l was found; the MEK level at that time point was 430 mg/l and rose to a maximum of 1050 mg/l 4 hours after the sBA administration.

DiVincenzo *et al.* (1976) examined the metabolism and clearance of MEK, the primary sBA metabolite, in serum of male guinea pigs following a single i.p. dose 450 mg/kg MEK as a 25% solution in corn oil. Metabolites were identified in serum by gas chromatography-mass spectrometry. The serum half-life of MEK was determined to be 270 minutes, and the clearance time was 12 hours. sBA, 3-hydroxy-2-butanone and 2,3-butanediol were identified as the serum metabolites of MEK. Reduction at the carbonyl group led to the formation of sBA from MEK. The sBA is then likely eliminated in urine as *o*-sulfates or *o*-glucuronide or may enter the intermediary metabolism to be eliminated as CO_2 or incorporated into tissues. Oxidation of MEK appeared to proceed by hydroxylation of the ω-1 carbon to form 3-hydroxy-2-butanone, which is further reduced to 2,3-butanediol (DiVincenzo *et al.*, 1976).

The following metabolic scheme is proposed (Figure 1):

Figure 1. Metabolic Pathways of sBA.



Dietz *et al.* (1981) developed a physiologically based pharmacokinetic model for sBA and its metabolites MEK, 3-hydroxy-2-butanone, and 2,3-butanediol in rats. The model examined the observed blood levels of sBA and the metabolites after oral administration of sBA, and was compared to blood levels of these compounds following oral exposure to MEK. The predicted blood concentrations of sBA and the metabolites were in good

agreement with observed data. The authors reported that that 97% of sBA administered orally at 1,776 mg/kgbw to rats was oxidized via alcohol dehydrogenase to MEK. Equimolar doses (1,776 mg/kg/bw) of sBA and MEK produced very similar maximum blood concentrations (Cmax) and areas under the concentration curve (AUC) for both MEK and 2,3-butanediol (Table 2).

Table 2. Blood Parent and Metabolite Concentrations after Administration of sBA and MEK to Rats.

	Parent and Metabolite Concentrations Following Oral sBA Dose[a]			
	sBA	**MEK**	**3-Hydroxy-2-butanone**	**2,3-Butanediol**
PEAK at time after dosing (mg/ml)	0.59 (2 hr)	0.78 (8 hr)	0.04 (12 hr)	0.21 (18 hr)
AUC (mg hr/L)	3254	9868	443	3167
	Parent and Metabolite Concentrations Following Oral MEK Dose[b]			
	MEK	**sBA**	**3-Hydroxy-2-butanone**	**2,3-Butanediol**
PEAK at time after dosing (mg/ml)	0.95 (4 hr)	0.033 (6 hr)	0.027 (8 hr)	0.26 (18 hr)
AUC (mg hr/L)	10, 899	414	382	3863

[a] 1,776 mg sBA/kg, or 2.2 ml/kg of a 22% aqueous solution
[b] 1,690 mg MEK/kg, or 2.1 ml/kg of a 21% aqueous solution
PEAK Maximum concentration measured
AUC Area under the concentration curve

In addition, human study data are available. The kinetics of inhaled MEK has been studied in human volunteers exposed in an exposure chamber (Liira *et al.*, 1988). Nine healthy males were exposed to 200 ppm MEK for 4 hours on two separate occasions, one with only sedentary activity and one that included three 10-minute periods of exercise. Relative pulmonary uptake of about 53% was found throughout a 4-hour inhalation exposure period. Blood MEK concentrations rose steadily throughout the exposure period without achieving a steady state. Exercise increased the overall blood MEK level markedly in comparison to sedentary activity. Only 2-3% of the absorbed dose was excreted unchanged by exhalation. This value is much lower than the pulmonary excretion observed after an oral dose of MEK (30%) by Munies and Wurster (1965).

The metabolite 2,3-butanediol, which was reported in the animal studies, was also detected in the urine of humans with maximum rates of excretion at about 6-12 hours from the beginning of exposure. About 2% of the absorbed MEK were excreted in the urine as 2,3-butanediol. The main portion of the inhaled MEK appears to be metabolized via pathways of the intermediary metabolism, e.g. converted to acetate or acetoacetate via the 3-hydroxy-2-butanone intermediate metabolite.

Health

The data on metabolism and pharmacokinetics of sBA in animals indicate that this chemical is rapidly absorbed, partly excreted as conjugates, but mostly metabolized to MEK. The MEK is subsequently converted to metabolites that are exhaled, excreted in the urine, or incorporated into endogenous metabolism. Based on this metabolic relationship, the toxicities of sBA and MEK in animals are considered to be very similar. It is assumed that the metabolic relationship between sBA and MEK in humans will be similar to that in rats.

sBA has a low order of acute toxicity to mammals. Oral LD_{50} values in laboratory animals range from approximately 2.2 to 6.5 g/kg body weight. The dermal LD_{50} value for sBA in rats was greater than 2 g/kg body weight. The inhalation LC_{50} for sBA is between 8,000 and 16,000 ppm for a 4-hr exposure. sBA liquid is practically non-irritating to the skin, but corrosive to the rabbit eye. It is a weak irritant to the respiratory tract of mice. sBA is not a skin sensitizer in animal studies.

In the Aarstad (1985) study, inductions of cytochrome P-450 concentrations were found in the livers (33% increase) and kidneys (47% increase) of rats that inhaled, 2,000 ppm sBA vapors for 3 days and 500 ppm vapors for 5 days, respectively. Information on repeated-dose toxicity of sBA can be deduced from a two-generation reproductive toxicity study (Cox *et al.*, 1975; Gallo *et al.*, 1977). sBA was initially administered to the F0 generation at concentrations of 0, 0.3, 1.0, and 3.0% in the drinking water. Due to toxicity at the 3%, the highest dose level; was reduced to 2.0% for the second-generation (F1 30/sex/group) that was reared to maturity (up to week 12), mated to produce a F2 generation, then sacrificed for organ weights, and gross and microscopic pathological evaluations. Ten F1 animals/sex/group were evaluated for hematological, biochemical, and urinary parameters at termination. A series of mild changes in the kidney (non-reactive tubular degeneration, tubular casts, foci of tubular regeneration, microcysts) were observed in animals treated with 2.0% sBA. The authors concluded that these findings were non-specific effects due to increased renal workload, possibly from an increased urine volume and pressure at the high dose of sBA. These effects were not considered to be a result of direct toxicity and did not have clear pathologic significance. No significant findings were seen. The no-effect level for the study was 1.0% (estimated to be approximately 1500 mg/kg/day by the authors and 1771 mg/kg/day by EPA/IRIS). The most comprehensive repeated-dose toxicity study available for MEK was conducted in rats by Cavender *et al.* (1983). None of the exposure concentrations (1,250, 2,500, or 5,000 ppm MEK vapor for 6 hours per day, 5 days per week, for 90 days) were lethal or even significantly harmful. There were no adverse effects on the clinical health or growth of male or female rats except a depression of mean body weight in the 5,000 ppm group. The female rats exposed to 5,000 ppm for 90 days showed only slightly increased liver weight, slightly decreased brain and spleen weights, and slightly altered blood chemistry in comparison with

controls. Male rats that received this exposure exhibited only a slightly increased liver weight. At the lower concentrations (1,250 and 2,500 ppm), there was only slightly increased liver weight for female rats and no significant differences for males. The pathological examination did not reveal any lesions that could be attributed to MEK exposure. The liver changes found in the study, an increase in liver weights and altered serum enzyme activities, indicate a MEK treatment-related effects; however, since histopathological lesions were not observed, these responses may have been the result of a physiologic adaptation mechanism. There were no findings of respiratory tract irritation in this study.

Additional information on repeated-dose effects by inhalation may be gained from a modified developmental study by Nelson *et al.* (1989). Rats were exposed by inhalation to 0, 3,500, 5,000 or 7,000 ppm sBA, 7 hours/day on days 1-19 of gestation and at 7,000 ppm, narcosis was observed in all animals. At 5000 ppm, the dams were partially narcotized with locomotion activity impaired. Maternal weight gain and food consumption was significantly reduced in all dose groups. The number of live fetuses was significantly reduced and resorptions were increased in the high exposure group only. Fetal body weights were significantly reduced in the mid- and high dose groups. There was no evidence of teratogenic effects in this study, and there was also no evidence of selective developmental toxicity. The no-effect levels were < 3,500 ppm for maternal toxicity and 3,500 ppm for developmental toxicity. In a two-generation reproductive toxicity study (Cox *et al.*, 1975; Gallo *et al.*, 1977), all findings at 0.3 and 1.0% were negative in both generations with respect to signs of toxicity in terms of growth and reproduction efficiency. In the group exposed to 3.0%, there were reductions in body weight gain during the 8-week pre-mating period, in number of pups born, and in pup body weight, but fertility was not affected. Due to toxicity, the high level was reduced to 2.0% for the second generation. In the second generation, the high level caused a slight but not significant depression in growth of weanling rats. The no-effect level for reproduction parameters was 1.0% (estimated to be 1500 mg/kg/day by the authors, and 1771 mg/kg/day by EPA/IRIS). Overall the weight of evidence indicates that sBA does not produce reproductive or teratogenic toxic effects in the developing embryo/fetus of laboratory animals.

sBA was inactive in *in vitro* tests for mutagenicity in both bacteria and yeast in either the presence or absence of metabolic activation (Brooks *et al.*, 1988; Elf Atochem, 1989). There was no structural damage to chromosomes observed in cultured mammalian cells (Chinese hamster ovary) treated with sBA (Brooks *et al.*, 1988). An evaluation of MEK in *in vivo* genotoxicity provides additional information on the potential for genotoxicity of sBA *in vivo*. MEK did not cause an increase in micronucleated polychromatic erythrocytes in two *in vivo* assays. MEK was also negative in the mouse lymphoma test, the chromosome aberration assay, and liver hepatocyte unscheduled DNA synthesis assay, MEK produces minimal or no systemic effects in laboratory animals following repeated exposure to high doses.

Acute Oral Toxicity

sBA has a low order of acute toxicity to mammals. The available data are reviewed below (Table 3). Clinical signs observed with acute intoxication following exposure to high levels of sBA in laboratory animals include variable expressions of central nervous system depression. Among the clinical effects reported were restlessness, ataxia,

prostration, decreased respiratory rate, narcosis and death. (Price, 1986; Hansen and Nielsen, 1994).

Table 3. Oral LD_{50} values for sBA.

Species and Exposure Condition	Result	Clinical Signs	Reference	CoR*
Rat, male Carworth-Wistar; diluted, 20%	LD_{50} = 6480 (5730-7320) mg/kg	Not reported	Mellon, 1951; Smyth *et al.*, 1954	2
Rat, male and female Fischer 344; undiluted sBA (99.5%); gavage dose - key study	LD_{50} = 2193 (1608-4146) mg/kg	Gait and/or posture abnormalities, coma, prostration	Price, 1986	1

* Criteria of reliability; see Appendix A

Acute Inhalation Toxicity

Studies by Mellon (1951) and Smyth *et al.* (1954) suggest that the LC_{50} for sBA is between 8,000 and 16,000 ppm for a 4-h inhalation exposure (Table 4). A vapor concentration of 10,000 ppm administered for 7 hours was lethal to rats (Nelson *et al.*, 1989).

Table 4. sBA Inhalation Toxicity Data.

Species and Exposure Condition	Result	Clinical Signs	Reference	CoR*
Rat, male and female Carworth-Wistar; 4-h exposure	16,000 ppm killed 5/6 rats	Not reported	Smyth *et al.*,1954	2
Rat, male and female Carworth-Wistar; 4-h exposure	8000 ppm killed 1/6 rats	Not reported	Mellon, 1951	2
Rat, female Sprague-Dawley; 7-h exposure	10,000 ppm killed 5/5 rats	Not reported	Nelson *et al.*, 1989	2

* Criteria of reliability; see Appendix A

Acute Dermal Toxicity

In an acute dermal toxicity study (Price, 1986), ten male and female Fischer 344 rats had sBA applied to the skin under an occlusive patch. Results of the study indicated no mortality at 2000 mg/kg and no clinical signs were observed.

Corrosiveness and Irritation

Skin Irritation

Using an OECD 404-test method, the skin irritation of sBA in white New Zealand rabbits was observed at 24, 48 and 72 hours and 7 days after dosing. Results indicate that sBA did not cause a skin reaction and is not considered a skin irritant in rabbits (Price, 1986).

Eye Irritation

Studies with rabbits using undiluted sBA liquid found moderate to severe irritation of the eyes (Table 5).

Table 5. sBA Eye Irritation Data.

Test Method	Test Conditions	Result	Reference	CoR*
OECD 405	0.1 ml of undiluted sBA (99.5%) instilled into the conjunctival sac of the eye	Moderate conjunctival inflammation in all six rabbits with slight, transitory iritic damage and/or corneal opacity in 3 rabbits. Intense, extensive corneal opacity and complete loss of iritic response developed in one rabbit.	Price, 1986	1
None	0.02 and 0.1 ml of undiluted sBA instilled into the conjunctival sac of the eye	Irritating Severe injury from 0.1 ml, minor from 0.02 ml	Mellon, 1952; Smyth *et al.*, 1954	2

* Criteria of reliability; see Appendix A

In the study of Price (1986), sBA was reported to be corrosive to the eye based on the progressive corneal opacity in one of six rabbits which was sacrificed at day 7. All other rabbits had mild effects but recovered completely by day 7.

Respiratory Tract Irritation

An Alarie test conducted in mice determined a RD_{50} value (concentration expected to cause a 50% decrease in respiratory rate over a 10-min exposure period) of 11,800 ppm for sBA vapor (Hansen and Nielsen, 1994).

Sensitization

sBA was not a skin sensitizer when tested in guinea pigs in Magnusson-Kligman maximization tests performed according to OECD guidelines (Price, 1986; Elf Atochem, 1997).

Repeated Dose Toxicity

There are several studies available that contribute to the weight of evidence regarding the repeated-dose toxicity of sBA. Many of the studies are limited in duration or

toxicological evaluation parameters. As a result, this endpoint is supplemented with data using an analog, methyl ethyl ketone (MEK).

Oral Toxicity

A two-generation reproductive toxicity study (Cox *et al.*, 1975) and a developmental toxicity study (Cox *et al.*, 1975) were conducted on sBA, which can also be considered relevant for repeat dose toxicity (Table 6).

Information on repeated-dose toxicity of sBA can be deduced from a two-generation reproductive toxicity study (Cox *et al.*, 1975; Gallo *et al.*, 1977). sBA was initially administered to the F0 generation at concentrations of 0, 0.3, 1.0, and 3.0% in the drinking water. Due to toxicity at the 3%, the highest dose level; was reduced to 2.0% for the second-generation (F1 30/sex/group) that was reared to maturity (up to week 12), mated to produce a F2 generation, then sacrificed for organ weights, and gross and microscopic pathological evaluations. Ten F1 animals/sex/group were evaluated for hematological, biochemical, and urinary parameters at termination. A series of mild changes in the kidney (non-reactive tubular degeneration, tubular casts, foci of tubular regeneration, microcysts) were observed in animals treated with 2.0% sBA. The authors concluded that these findings were non-specific effects due to increased renal workload, possibly from an increased urine volume and pressure at the high dose of sBA. These effects were not considered to be a result of direct toxicity and did not have clear pathologic significance. No significant findings were seen. The no-effect level for the study was 1.0% (estimated to be approximately 1500 mg/kg/day by the authors and 1771 mg/kg/day by EPA/IRIS).

Table 6. sBA Oral Repeated Dose Toxicity Data.

Species and Exposure Condition	Result	Clinical Signs	Reference	CoR*
Rat, male and female Wistar; 8-wks exposure	NOAEL F1 offspring = 1% (estimated 1500 mg/kg/day by authors and 1771 mg/kg/day in EPA IRIS)	Mild changes in kidney, but not specific and due to increased renal workload	Cox *et al.*, 1975; Gallo *et al.*, 1977	2
Rat, female Wistar; 8-wks exposure premating and during gestation	NOAEL maternal and pup = 1% (1771 mg/kg/day)	Fetotoxic at 2% (3122 mg/kg/day) showing decreased pup weights. Increase in missing sternebrae, wavy ribs, and incomplete vertebra ossification at 2%, but consistent in type and frequency with the controls and the spontaneous incidences in the colony. Effects were not determined to be compound-related.	Cox *et al.*, 1975 ; Gallo *et al.*, 1977	2

* Criteria of reliability; see Appendix A

Inhalation Toxicity

There is one inhalation repeated-dose (Aarstad *et al.*, 1985) and one developmental toxicity study (Nelson *et al.*, 1989) available on sBA. These studies are limited due to their short duration and limited evaluation of toxicological parameters. Further supportive data are available from a 90-day inhalation toxicity study conducted on MEK, the major initial metabolite of sBA (Table 7).

Studies were conducted primarily to assess narcosis, liver and kidney mixed function oxidases, and developmental toxicity. In the Aarstad study, inductions of cytochrome P-450 concentrations were found in the livers (33% increase) and kidneys (47% increase) of rats that inhaled, 2,000 ppm sBA vapors for 3 days and 500 ppm vapors for 5 days, respectively. The most comprehensive subchronic toxicity study available for MEK was conducted in rats by Cavender *et al.* (1983). In this study, male and female rats were exposed to 0, 1,250, 2,500, or 5,000 ppm MEK vapors for 6 hours per day, 5 days per week, for 90 days. The animals were examined for clinical signs of toxicity and changes on body weight, clinical pathology parameters (hematology and serum chemistry), gross pathology and histopathology, and neuropathology. The results of this study indicated that none of the MEK exposure concentrations were lethal or even significantly harmful. There were no adverse effects on the clinical health or growth of male or female rats except a depression of mean body weight in the 5,000 ppm group. The female rats

exposed to 5,000 ppm for 90 days showed only slightly increased liver weight, slightly decreased brain and spleen weights, and slightly altered blood chemistry in comparison with controls. Male rats that received this exposure exhibited only a slightly increased liver weight. At the lower concentrations (1,250 and 2,500 ppm), there was only slightly increased liver weight for female rats and no significant differences for males. The pathological examination did not reveal any lesions that could be attributed to MEK exposure. The liver changes found in the study, an increase in liver weights and altered serum enzyme activities, indicate a MEK treatment-related effect; however, since histopathological lesions were not observed, these responses may have been the result of a physiologic adaptation mechanism. There were no findings of respiratory tract irritation in this study. MEK produces minimal or no systemic effects in laboratory animals following repeated exposure to high doses. This finding is supported by a number of subchronic toxicity studies that were conducted using multiple experimental animal species and a variety of exposure routes (ATSDR, 1992; IPCS, 1993). The NOAEL is 5000 ppm.

Table 7. sBA Inhalation Repeated Dose Toxicity Data.

Species and Exposure Condition	Result	Clinical Signs	Reference	CoR*
Rat, male Sprague-Dawley; 3-d (2000 ppm), 5-d (500 ppm) exposure	47% and 33% increase in cytochrome P-450 at 500 and 2000 ppm, respectively		Aarstad *et al.*, 1985	2
Rat, female Sprague-Dawley; 19-d exposure	NOAEL maternal = 3500 ppm, NOAEL teratogen > 7000 ppm (highest dose tested)	Number of live fetuses significantly reduced and resorptions increased at 7000 ppm; fetal body weights significantly reduced at 3500 and 7000 ppm	Nelson *et al.*, 1989	2
Rat, male and female Fischer 344, 90-d exposure to MEK	NOAEL > 5000 ppm (highest dose tested)	Slight decreased brain and spleen weights, increased liver weight, and altered blood chemistry in females and slight increased liver weight in males. Since histopathological lesions were not observed, these responses may have been the result of a physiologic adaptation mechanism.	Cavender *et al.*, 1983	1

* Criteria of reliability; see Appendix A

Mutagenicity

Sufficient data are available for sBA to adequately characterize its *in vitro* genotoxicity. MEK data are used as an analog to address the endpoint for *in vivo* genotoxicity and supplement existing data on sBA data for *in vitro* genotoxicity.

***In Vitro* Genotoxicity**

Screening level mutagenic studies conducted for sBA indicate that this material is not genotoxic (Table 8). sBA was inactive in vitro tests for mutagenicity in both bacteria and yeast in either the presence or absence of metabolic activation (Brooks *et al.*, 1988; Elf Atochem, 1989). There was also no structural damage to chromosomes observed in cultured mammalian cells (Chinese hamster ovary) treated with sBA (Brooks *et al.*, 1988) (Table 8).

Available data on MEK indicate that MEK is negative in the mouse lymphoma assay, chromosomal aberration and cytotoxicity study, an unscheduled DNA synthesis and a morphologic transformation assay (Clone A31-1); (Table 9). These results are consistent with those determined using sBA.

Table 8. sBA Genotoxicity Data.

Endpoint and Test System	Test Conditions	Result / Toxicity	Geno-toxicity	Reference	CoR*
Gene mutation assay with *Salmonella typhimurium* TA98, TA100, TA1535, TA1537, and TA1538	Up to 10 mg/plate ± rat S9. Pre-incubation assay	Toxic at 10 mg/plate on TA100 without S9	No mutagenic activity	Elf Atochem, 1989	1
Gene mutation assay with *Salmonella typhimurium* TA98, TA100, TA1535, TA1537, and TA1538	Up to 4 mg/plate ± rat S9. Plate incorporation assay	No toxicity	No mutagenic activity	Brooks *et al.*, 1988	1
Gene mutation assay with *Escherichia coli* WP2 uvrA pKM101	Up to 4 mg/plate ± rat S9. Plate incorporation assay	No toxicity	No mutagenic activity	Brooks *et al.*, 1988	1
Gene conversion assay with *Saccharomyces cerevisiae* JD1	Up to 5 mg/ml ± rat S9	No toxicity	No mutagenic activity	Brooks *et al.*, 1988	1
Chromosomal aberration assay with cultured Chinese hamster ovary (CHO) cells	Up to 5 mg/ml ± rat S9	No toxicity	No clastogenic activity	Brooks *et al.*, 1988	1

* Criteria of reliability; see Appendix A

***In Vivo* Genotoxicity**

Data on sBA for in vivo mammalian genetic toxicity were not available and as a result, MEK data were used as an analog (O'Donoghue,1988; Basler, 1986). MEK did not cause an increase in micronucleated polychromatic erythrocytes in two in vivo assays as shown below in Table 9. Based on similarities between sBA and MEK, it is concluded that sBA will also be considered negative in these assay systems.

Table 9. MEK Mammalian Genetic Toxicity Data.

Test	Species	Study Design	Results	References
***In Vitro* Test**	Mouse lymphoma assay	L5178Y/TK +/-	Negative with and without activation	O'Donoghue *et al.*, 1988
	Rat liver cells	RL4 Chromosomal aberration and cytotoxicity	Negative with and without activation	Brooks *et al.*, 1988
	Rat hepatocyte	Unscheduled DNA synthesis	Negative with and without activation	O'Donoghue *et al.*, 1988
	Mouse BALB 3T3 cells	Morphologic transformation (Clone A31-1)	Negative with and without activation	O'Donoghue *et al.*, 1988
In Vivo	Mouse	Micronucleus Assay i.p. injection	Negative	O'Donoghue *et al.*, 1988
In Vivo	Hamster	Micronucleus Assay i.p. injection	Negative	Basler, 1986

Reproductive Toxicity

In a two-generation reproductive toxicity study (Cox *et al.*, 1975; Gallo *et al.*, 1977), sBA was initially administered via drinking water at concentrations of 0, 0.3, 1.0, and 3.0% to male and female rats (Table 10). All findings at 0.3 and 1.0% were negative in both generations with respect to signs of toxicity in terms of growth and reproduction efficiency. In the group exposed to 3.0%, there were reductions in body weight gain during the 8-week pre-mating period, in number of pups born, and in pup body weight, but fertility was not affected. Due to toxicity, the high dose level was reduced to 2.0% for the second generation. In the second generation, the high dose level caused a slight but not statistically significant depression in growth of weanling rats. The maternal and pup no-effect levels for reproduction parameters were 1.0% (estimated to be 1500 mg/kg/day by the authors, and 1771 mg/kg/day by EPA/IRIS). Overall, the weight of evidence indicates that sBA does not produce reproductive effects.

Table 10. sBA Oral Reproductive Toxicity Data.

Species and Exposure Condition	Result	Clinical Signs	Reference	CoR*
Rat, male and female Wistar; 8-wks exposure	NOAEL F1 offspring = 1% (estimated 1500 mg/kg/day by authors and 1771 mg/kg/day in EPA IRIS)	Mild changes in kidney, but not specific and due to increased renal workload	Cox *et al.*, 1975; Gallo *et al.*, 1977	2

* Criteria of reliability; see Appendix A

Developmental Toxicity

Developmental effects, such as delayed development, have been produced in laboratory animals with sBA, but only at doses that were maternally toxic. Overall the weight of evidence indicates that sBA does not produce teratogenic (developmental) toxic effects in the developing embryo/fetus of laboratory animals (Table 11).

Oral Route

During the two-generation reproductive toxicity (see section 3.6) a teratogenic phase was incorporated in which the parents (28-30/group) were rebred to produce a second litter. The females were subjected to Caesarean section on day 20 of gestation (Cox *et al.*, 1975; Gallo *et al.*, 1977). At 2.0%, sBA caused a significant depression in fetal weight, with evidence of delayed skeletal maturation, but no skeletal and visceral malformations. The authors concluded that these changes represented mild toxicity and were reminiscent of stress lesions. All findings at 0.3 and 1.0% were negative. The no-effect level for developmental toxicity was 1.0% (estimated to be 1500 mg/kg/day by the authors and 1771 mg/kg/day by EPA/IRIS].

Inhalation Route

In a developmental toxicity study (Nelson *et al.*, 1989) groups of 15-16 pregnant rats were exposed via inhalation to 0, 3,500, 5,000 or 7,000 ppm sBA, 7 hours/day on days 1-19 of gestation; the dams were sacrificed on day 20. At 7,000 ppm, narcosis was observed in all animals. At 5000 ppm, the dams were partially narcotized with locomotion activity impaired. Maternal weight gain and food consumption was significantly reduced in all dose groups. The number of live fetuses was significantly reduced and resorptions were increased in the high exposure group only. Fetal body weights were significantly reduced in the mid- and high dose groups. There was no evidence of teratogenic effects in this study, and there was also no evidence of selective developmental toxicity. For maternal toxicity the NOEL was < 3,500 ppm (10,593 mg/m^3) with a NOAEL of 3,500 ppm. For developmental toxicity, the NOEL was 3500 ppm with a NOAEL of >7000 ppm (21,186 mg/m^3).

Table 11. sBA Developmental Toxicity Data.

Species and Exposure Condition	Result	Clinical Signs	Reference	CoR*
Rat, female Wistar; 8-wks exposure premating and during gestation; oral	NOAEL maternal and pup = 1% (1771 mg/kg/day)	Fetotoxic at 2% (3122 mg/kg/day) showing decreased pup weights. Increase in missing sternebrae, wavy ribs, and incomplete vertebra ossification at 2%, but consistent in type and frequency with the controls and the spontaneous incidences in the colony. Effects were not determined to be compound-related.	Cox *et al.*, 1975 ; Gallo *et al.*, 1977	2
Rat, female Sprague-Dawley; 19-d exposure; inhalation	NOAEL maternal = 3500 ppm, NOAEL teratogen > 7000 ppm (highest dose tested)	Number of live fetuses significantly reduced and resorptions increased at 7000 ppm; fetal body weights significantly reduced at 3500 and 7000 ppm	Nelson *et al.*, 1989	2

* Criteria of reliability; see Appendix A

Other Toxicological Endpoints

Neurotoxicity

sBA, like many other organic solvents, produces reversible depression of central nervous system (CNS) activity in laboratory animals at high exposure doses (Snyder and Andrews 1996). Laboratory animals that were exposed to acutely toxic doses of sBA exhibited clinical signs of CNS depression that were reversible in survivors upon termination of exposure. One limited acute neurotoxicity study in laboratory animals is reported for sBA. In a simple functional test, the tilted plane test was used to evaluate rats that received a single oral dose of sBA and the results were compared with analogous doses of ethanol, propanols, and other butanols (Wallgren, 1960). An sBA dose of 0.0163 mole/kg (approximately 1.2 g/kg) is found to produce a greater intoxication effect than ethanol (relative molar intoxicating effect values of 4.4 and 1 for sBA and ethanol, respectively) and a slower recovery to normal behavior than ethanol.

There are several *in vitro* neurological studies that included sBA among groups of alcohols tested to examine neurological mechanisms of acute alcohol intoxicating effects (Lyon *et al.*, 1981; Rand and Li, 1994; Tanii *et al.*, 1995). These studies, however, are of low value in assessing functional neurological effects associated with acute sBA exposure.

The potential for neurotoxicity associated with repeated exposure to sBA has not been specifically evaluated. sBA caused partial narcosis at 5,000 ppm in pregnant rats in the developmental toxicity study by Nelson *et al.* (1989) discussed above. The few repeated exposure studies that have been conducted for sBA did not indicate enduring adverse effects on the nervous system of laboratory animals; however, the experimental designs of these studies do not permit definitive assessment.

Other Effects

sBA has demonstrated activity in a number of physiology and interaction studies. sBA inhibited the contraction of the depolarized guinea pig ileum inducted by calcium chloride (Yashuda *et al.*, 1976); produced an increase in cyclic AMP in human peripheral lymphocytes (Atkinson *et al.*, 1977), enhanced microsomal enzymes and metabolism (Aarstad *et al.*, 1985; Traiger *et al.*, 1989; Page and Carlson, 1993; Gadberry and Carlson, 1994) and potentiated the toxicity of carbon tetrachloride (Cornish and Abefuin, 1967). The experimental designs of these studies, however, limit their application to the hazard assessment of sBA.

Toxicity Data for Diisopropyl Ether

A test plan and dossier for diisopropyl ether (DIPE) have been submitted to the U.S. EPA by the Isopropanol Panel of the American Chemistry Council (2006). DIPE is a small molecular weight ether similar in structure to sBE and the mammalian toxicity data identified for DIPE can be used as an analog to support the characterization of mammalian toxicity for sBE, as their inherent toxicities are expected to be similar. The complete dossier for DIPE is provided with this test plan. The HPV endpoints for DIPE are characterized in Table 12 and the study summaries can be found in the dossier, which is provided with this test plan.

Table 12. Mammalian Toxicity Data for DIPE.

Toxicity Endpoint		Results	Reference
Acute	Inhalation	Low toxicity	Kimura *et al*., 1971 Machle *et al.,* 1939
	Oral	Low toxicity	Kimura *et al*., 1971 Machle *et al.,* 1939
	Dermal	Low toxicity	Kimura *et al*., 1971 Machle *et al.,* 1939
Irritation	Skin	Minimal irritant	Machle *et al*., 1939
	Eye	Minimal irritant	Machle *et al*., 1939
	Respiratory	Sensory irritant	Hine *et al*., 1955 Silverman *et al*., 1946
Sensitization		Negative *in vitro* sensitizer	Wass and Belin, 1990
Repeated Dose		Liver and kidney effects	Dalbey and Feuston, 1996
Reproductive		No effects on reproductive organ structure or sperm/spermatid number	Dalbey and Feuston, 1996
Developmental		Equivocal developmental effect at maternal effect level	Dalbey and Feuston, 1996
Neurotoxicity		Minor reversible effect on CNS	Rodriguez and Dalbey, 1997
Geno-toxicity	*In vitro* mutation	Negative	Brooks *et al*., 1988
	In vitro chromosome aberration	Negative	Brooks *et al*., 1988

C. Aquatic Toxicity Data

Although experimental data were not available to characterize the acute aquatic toxicity of sBE to fish, invertebrates, and green algae, a Quantitative Structure Activity Relationship (QSAR) model that applies an equation for neutral organics to estimate aquatic toxicity is appropriate for sBE. Modeling was performed using the ECOSAR computer model (Cash and Nabholz, 1990). ECOSAR is a subroutine of the EPI Suite™ computer model. Results of modeling show that sBE is expected to exhibit a 96-hour LC_{50} value of 14.7 mg/l for a freshwater fish, a 48-hour EC_{50} value of 16.7 mg/l for a daphnid (freshwater invertebrate), and a 96-hour EC_{50} value of 11.0 mg/l for a green alga (Table 13). Based on these model values, sBE presents a moderate order of acute toxicity to aquatic species. Table 13 also shows modeled chronic data for a fish, invertebrates, and green algae. The values for both sBE and nBE range from approximately 1 to 2 mg/L for the three trophic levels.

There are measured and calculated data for an analog ether, n-butyl ether (nBE; CAS No. 142-96-1), that support using the calculated data for sBE. A study that evaluated nBE acute toxicity to fish was reported by the Ministry of International Trade and

Industry of Japan (CITI, 1992). The study reported a 48-hour LC_{50} value of 30.7 mg/l for the Orange Killifish (*Oryzias latipes*). The modeled 96-hour LC_{50} value for nBE was 10.8 mg/l for a freshwater fish. The difference in exposure periods can explain some of the difference between the two values. However, a comparison of the two values supports the use of the ECOSAR model to estimate aquatic toxicity for these chemicals and suggest that the modeled data may be conservative.

Table 13. Calculated Aquatic Toxicity Data for sBE and nBE.

Endpoint	Result (mg/l)	
	sBE	**nBE**
Acute		
Fish 96-hr LC_{50}	14.7	10.8 (30.7*)
Daphnid 48-hr EC_{50}	16.7	12.5
Alga 96-hr EC_{50}	11.0	8.3
Chronic		
Fish 30-da ChV**	2.2	1.6
Daphnid 16-da EC_{50}	1.3	1.0
Alga 96-hr ChV**	1.8	1.5

* Experimental 48-hour LC_{50} (CITI, 1992)
** Chronic Value

D. Environmental Fate Data

Biodegradation

Biodegradation of an organic substance by bacteria can provide energy and carbon for microbial growth. This process results in a structural change of an organic substance and can lead to the complete degradation of that substance, producing carbon dioxide and water.

Experimental data are not available to assess the biodegradability of sBE. However, a number of published studies in which non-standard guideline methods were used have demonstrated that alkyl ethers can be degraded by pure strains and mixed cultures of bacteria when incubated under aerobic conditions (Fujiwara, *et al.*, 1984; Kim and Engesser, 2004). The rate of biodegradation for these substances is slow because it is believed the ether bond has high dissociation energy (about 360kJ mol^{-1}) (Kim and Engesser, 2004). A modified MITI test conducted on the analog substance nBE reported a 28-day percent biodegradation of 3 to 4%, based on biological oxygen demand (CITI, 1992). The BIOWIN model, a subroutine within the EPI Suite (2000) computer model, further supports this and estimates biodegradation of both sBE and nBE to occur at a slow rate.

Photodegradation – Photolysis

Direct photochemical degradation occurs through the absorbance of solar radiation by a

chemical substance in aqueous solution. If the absorbed energy is high enough, then the resultant excited state of the chemical may undergo a transformation. A prerequisite for direct photodegradation is the ability of one or more bonds within a chemical to absorb ultraviolet (UV)/visible light in the 290 to 750 nm range. Light wavelengths longer than 750 nm do not contain sufficient energy to break chemical bonds, and wavelengths below 290 nm are shielded from the earth by the stratospheric ozone layer (Harris, 1982a).

An approach to assessing the potential for a substance to undergo photochemical degradation is to assume that degradation will occur in proportion to the amount of light wavelengths >290 nm absorbed by constituent molecules (Zepp and Cline, 1977).

Saturated hydrocarbons and R-OH groups do not absorb light above 290 nm (Harris, 1982a). Therefore, these moieties are stable in regard to direct photolytic processes. Ethers are also stable as this group absorbs UV light in the far UV region, below 220 nm (Mill, 2000). Therefore, direct photolysis will not be an important transformation process for the degradation of sBE in the environment.

Photodegradation – Atmospheric Oxidation

Photodegradation can be measured (U.S. EPA, 1999a) or estimated using an atmospheric oxidation potential (AOP) model accepted by the EPA (U.S. EPA, 1999b). Atmospheric oxidation as a result of hydroxyl radical attack is not direct photochemical degradation, but rather indirect degradation.

sBE has the potential to volatilize to air, based on a vapor pressure of 21.7 hPa @ 25º C, where it is subject to atmospheric oxidation. In air, sBE can react with photosensitized oxygen in the form of hydroxyl radicals ($^{\bullet}OH$). The computer program AOPWIN (atmospheric oxidation program for Microsoft Windows) (EPI Suite, 2000) calculates a chemical half-life for a 12-hour day based on an $^{\bullet}OH$ reaction rate constant and a defined $^{\bullet}OH$ concentration (the 12-hour day half-life value normalizes degradation to a standard day light period during which hydroxyl radicals needed for degradation are generated).

sBE has a calculated half-life in air of 4.0 hours or 0.33 days, based on a rate constant of 3.21E-13 cm^3/molecule*sec and an $^{\bullet}OH$ concentration of 1.5E6 $^{\bullet}OH$ /cm^3.

Stability in Water (Hydrolysis)

Hydrolysis of an organic chemical is the transformation process in which a water molecule or hydroxide ion reacts to form a new carbon-oxygen bond. Chemicals that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (Neely, 1985). The lack of a suitable leaving group renders a compound resistant to hydrolysis. sBE is expected to be resistant to hydrolysis because it lacks a functional group that is hydrolytically reactive (Harris, 1982b). Therefore, hydrolysis will not contribute to its removal from the environment.

Chemical Distribution In The Environment (Fugacity Modeling)

Fugacity-based multimedia modeling provides basic information on the relative distribution of a chemical between selected environmental compartments. Two widely used fugacity models are the EQC (Equilibrium Criterion) Level I and Level III model

(Mackay *et al.*, 1996; Mackay *et al.*, 2003). The Mackay Level I and Level III Models do not include a groundwater compartment.

The input data required to run a Level I model include basic physicochemical parameters; distribution is calculated as the percent of chemical partitioned to six compartments (air, soil, water, suspended sediment, sediment, biota) within a unit world. Level I data are basic partitioning data that allow for comparisons between chemicals and indicate the compartment(s) to which a chemical may partition, based on the selected physical parameters. The Level III model uses the same physical parameters as the Level I model, but also requires half-life degradation data for the air, soil, water, and sediment compartments, as well as emission parameters for the air, water, and soil compartments. Distribution in the Level III model is calculated as percent of chemical partitioned to 4 compartments (air, water, soil and sediment) within a unit world. As with Level I data, Level III data are basic partitioning data that allow for comparisons between chemicals and indicate the compartment(s) to which a chemical may partition.

Results of the Mackay Level I environmental distribution model (Table 14) suggest that sBE will partition primarily to the air (>99%). These results can be largely explained by its vapor pressure, 2170 Pa at 25°C, one of the physical parameters used by the model. In comparison, the Level III model suggests that the majority of sBE will partition primarily to the soil (51%) and water (45%) compartments (Table 15).

Table 14. Environmental Distribution as Calculated by the Mackay (2003) Level I Fugacity Model.

Environmental Compartment	Percent Distribution*
Air	99.1
Water	0.5
Soil	0.4
Sediment	<0.01
Suspended Sediment	<0.01
Biota	<0.01

* Distribution is based on the following model input parameters for sBE:

Molecular Weight	130.23
Temperature	25°C
Log K_{ow}	2.87
Water Solubility	327 g/m^3
Vapor Pressure	2170 Pa
Melting Point	-100°C

Table 15. Environmental Distribution as Calculated by the Mackay (2003) Level III Fugacity Model.

Environmental Compartment	Percent Distribution*
Air	3.2
Water	44.8
Soil	51.1
Sediment	0.9

* Distribution is based on the following model input parameters for sBE:

Molecular Weight	130.23	Degradation half-lives:	
Temperature	25°C	Air	4.0 hrs
Log K_{ow}	2.87	Water	320 hrs
Water Solubility	327 g/m^3	Soil	7200 hrs
Vapor Pressure	2170 Pa	Sediment	72000 hrs
Melting Point	-100°C		

Bioaccumulation Potential

A bioconcentration factor (BCF) of 32 (log BCF = 1.5) is calculated for sBE (EPI Suite, 2000) using a log K_{ow} value of 2.87. These data indicate that sBE has a low BCF and is not expected to bioaccumulate. Additionally, a 6-week BCF study, conducted by the Ministry of International Trade and Industry of Japan, reported a measured BCF in carp (*Cyprinus carpio*) of 47 to 83 for nBE (CITI, 1992). Computer model estimates for nBE indicate a BCF of 59 using a log K_{ow} value of 3.21. These data support the use of the calculated BCF value for sBE.

IV. TEST PLAN AND DATA SUMMARY FOR sBE

A search for existing studies/information and their review identified good quality data to characterize the hazard of sBE for all endpoints in the U.S. HPV Program. Where there were good quality data for selected endpoints beyond those included in the HPV Program, they were added to their respective dossiers.

Three dossiers are forwarded with this test plan. They include sBE, DIPE, and sBA. Data for MEK are included in the sBA dossier. No further testing is planned. Data to characterize the endpoints discussed in this test plan for sBE are summarized in Table 16.

Table 16. Data Characterizing Endpoints for sBE.

Endpoint	Characterization / Value	Source
Physicochemical		
Melting Point (ºC)	-100 (m)	EPI Suite, 2000
Boiling Point (ºC)	116 (c)	EPI Suite, 2000
Vapor Pressure (hPa @ 25ºC)	21.7 (m)	EPI Suite, 2000
Water Solubility (mg/L@ 25ºC)	327 (c)	EPI Suite, 2000
Log K_{ow} (25ºC)	2.87 (c)	EPI Suite, 2000
Environmental Fate		
Biodegradation	Slow (m, c)	EPI Suite, 2000 Fujiwara, *et al.*, 1984 Kim and Engesser, 2004
Direct Photolysis	Direct photolysis will not contribute to degradation	Harris, 1982a Mill, 2000 Zepp and Cline, 1977
Indirect Photolysis (half- life; da)	0.33 (c)	EPI Suite, 2000
Hydrolysis	Hydrolysis will not contribute to degradation	Harris, 1982b Neely, 1985
Fugacity - Level I (Distribution to compartment)	Partitions primarily to: air (>99%) (c)	Mackay *et al.*, 1996 Mackay *et al.*, 2003
Fugacity - Level III (Distribution to compartment)	Partitions primarily to: soil (51%); water (45%) (c)	Mackay *et al.*, 1996 Mackay *et al.*, 2003
Aquatic Toxicity		
Freshwater Fish 96-hr LC_{50} (mg/L)	14.7 (c)	Cash and Nabholz, 1990
Freshwater Fish 30-da ChV* (mg/L)	2.2 (c)	Cash and Nabholz, 1990
Freshwater Invert. 48-hr EC_{50} (mg/L)	16.7 (c)	Cash and Nabholz, 1990
Freshwater Invert. 16-da EC_{50} (mg/L)	1.3 (c)	Cash and Nabholz, 1990
Freshwater Alga 96-hr EC_{50} (mg/L)	11.0 (c)	Cash and Nabholz, 1990
Freshwater Alga 96-hr ChV* (mg/L)	1.8 (c)	Cash and Nabholz, 1990

Table 16 (continued). Data Characterizing Endpoints for sBE.

Endpoint		Characterization / Value	Source
Mammalian Toxicity			
Acute	Inhalation	Low toxicity LD_{50} = >8,000 ppm (4 hr) LD_{50} = <16,000 ppm (4 hr) (ra from sBA) (m)	Mellon, 1951 Smyth *et al.*,1954
	Oral	Low toxicity LD_{50} = 2.2 to 6.5 g/kg bw (ra from sBA) (m)	Mellon, 1951 Smyth *et al.*, 1954 Price, 1986
	Dermal	Low toxicity LD_{50} = >2 g/kgbw (ra from sBA) (m)	Price, 1986
Irritation	Skin	Minimal irritant PII = 0 (ra from sBA) (m)	Price, 1986
	Eye	Moderate – Severe irritant (ra from sBA) (m)	Mellon, 1952 Smyth *et al.*, 1954 Price, 1986
	Respiratory	640 ppm RD_0 Threshold at 2 Min, 11800 ppm RD_{50} at 10 Min (ra from sBA) (m)	Hansen and Nielsen, 1994
Sensitization		Negative sensitizer (ra from sBA) (m)	Price, 1986 Elf Atochem, 1997
Repeated Dose		Oral sBA NOEL = 1.0% (1771 mg/kg/day); Inhalation MEK NOAEL = 5000 mg/kg/day (ra from sBA and MEK) (m)	Cox *et al.*, 1975 Cavender *et al.*, 1983
Reproductive		Not a Reproductive Hazard NOAEL = 1771 mg/kg/day (ra from sBA) (m)	Cox *et al.*, 1975 Gallo *et al.*, 1977
Developmental		Oral NOEL (maternal) = 1771 mg/kg/day NOEL (pup) = 1771 mg/kg/day Inhalation NOEL (maternal) = <3,500 ppm NOAEL (maternal) = 3,500 ppm NOEL (pup) = 3,500 ppm NOAEL (pup) = >7,000 ppm (ra from sBA) (m)	Cox *et al.*, 1975 Gallo *et al.*, 1977 Nelson *et al.*, 1989

Table 16 (continued). Data Characterizing Endpoints for sBE.

Endpoint		Characterization / Value	Source
Mammalian Toxicity			
Neurotoxicity		Minor reversible narcosis at 5,000 ppm in pregnant rats in the developmental toxicity study (ra from sBA) (m)	Nelson *et al.*, 1989
Geno-toxicity *In vitro*	Mutation	*S. typhimurium* Negative *E. coli* Negative (ra from sBA) (m)	Brooks *et al*., 1988
	Chromosome aberration	Chinese hamster ovary Negative (ra from sBA) (m)	Brooks *et al*., 1988
	Gene conversion assay	*S. cerevisiae* Negative (ra from sBA) (m)	Brooks *et al*., 1988
	Mouse lymphoma	L5178Y/TK +/- Negative with and without activation (ra from MEK) (m)	O'Donoghue *et al.*, 1988
	Rat liver cells chromosomal aberration and cytotoxicity	RL4 Negative with and without activation (ra from MEK) (m)	Brooks *et al.*, 1988
	Rat hepatocyte unscheduled DNA synthesis	Negative with and without activation (ra from MEK) (m)	O'Donoghue *et al.*, 1988
	Morphologic transformation (Clone A31-1)	Mouse BALB 3T3 cells Negative with and without activation (ra from MEK) (m)	O'Donoghue *et al.*, 1988
Geno-toxicity *In vivo*	Mouse Micronucleus Assay i.p. injection	Negative (ra from MEK) (m)	O'Donoghue *et al.*, 1988
	Hamster Micronucleus Assay i.p. injection	Negative (ra from MEK) (m)	Basler, 1986

m Measured for sBE
c Calculated for sBE
ra Read-across data from analog and/or metabolite as indicated
* Chronic value

REFERENCES

Aarstad K, Zahlsen K and Nilsen O (1985). Inhalation of butanols, changes in the cytochrome P-450 enzyme system. Arch. Toxicol. (suppl.) 8:418-421.

Atkinson J, Sullivan T, Kelly J and Parker C (1977). Stimulation by alcohols of cyclic AMP metabolism in human leukocytes. J. Clin. Invest. 60:284-294.

ATSDR (Agency for Toxic Substances and Disease Registry) (1992). Toxicological profile for 2-butanone. PB93-110708.

Basler A (1986). Aneuploidy-inducing chemicals in yeast evaluated by the micronucleus test. Mut. Res. 174:11-13.

Brooks T, Meyer A and Hutson D (1988). The genetic toxicology of some hydrocarbon and oxygenated solvents. Mutagenesis. 3:227-231.

Cash G and Nabholz V (1990). ECOSAR. U.S. Environmental Protection Agency, Office of Pesticide, Pollution, and Toxics - Risk Assessment Division. Washington, DC, USA.

Cavender F, Casey H, Salem H, Swenberg J, and Gralla E (1983). A 90-day vapor inhalation toxicity study of methyl ethyl ketone. Fund. Appl. Toxicol. 3:264-270.

Chemicals Inspection and Testing Institute (CITI) (1992). Biodegradation and bioaccumulation data of existing chemicals based on the CSCL Japan. CITI (ed.). Chemical Products Safety Division, Basic Industries Bureau, Ministry of International Trade and Industry, Japan. Japan Chemical Industry Ecology-Toxicology and Information Center.

Cornish H and Abefuin J (1967). Potentiation of carbon tetrachloride toxicity by aliphatic alcohols. Arch. Environ. Health. 14:447-449.

Cox G, Bailey D and Morgareidge K (1975). Toxicity studies in rats with 2-butanol including growth, reproduction, and teratologic observation. Food and Drug Research Laboratories. LaB No. 2093. Astra Nutrition, Molndal Sweden [with TSCE 8(e) cover note dated May 11, 1992 by Shell Oil, Houston, TX, USA].

Dalbey W and Feuston M (1996). Subchronic and developmental toxicity studies of vaporized diisopropyl ether. J. Toxicol. Environ. Health. 49:29-43.

Dietz F, Rodriguez-Giaxola M, Traiger G, Stella V and Himmelstein K (1981). Pharmocokinetics of 2-butanol and its metabolites in the rat. J. Pharmokinet. Biopharm. 9:533-576.

DiVincenzo G, Kaplan C and Dedinas J (1976). Characterization of the metabolites of methyl n-butyl ketone, methyl iso-butylketone, and methyl ethyl ketone in guinea pig serum and their clearance. Toxicol. Appl. Pharm. 36:511-522.

ECOSAR v0.99h (2004) in EPI Suite™ (2000). Estimation Program Interface Suite, v3.12. Syracuse Research Corporation, Syracuse, NY, USA.

Elf Atochem (1989). Butanol secondaire. Test d'Ames «Essai de mutation réverse sur Salmonella typhimurium». Sanofi Recherche, Report No. RS860890421/JV2.

Elf Atochem (1997). Skin sensitization test in guinea pigs (maximization method of Magnusson and Kligman) with sec-butanol. CIT report no.14861 TSG.

EPI Suite™ (2000). Estimation Program Interface Suite, version 3.12. Syracuse Research Corporation, Syracuse, NY, USA.

Fujiwara Y, Kinoshita T, Sato H, Kojima I. (1984) Biodegradation and Bioconcentration of Alkyl Ethers. Yukagaku, 33: 111-114.

Gadberry M, and Carlson G (1994). 2-Butanol metabolism by rat hepatic and pulmonary cytochromes P450. Toxicol. Letters. 74:203-209.

Gallo M, Oser B, Cox G and Bailey D (1977). Studies on the long-term toxicity of 2-butanol. Toxicol. Appl. Pharmacol. 41:135. [Abstract]

Hansen L and Nielsen G (1994). Sensory irritation, pulmonary irritation and structure-activity relationships of alcohols. Toxicol. 88:81-99.

Harris J (1982a). Rate of aqueous photolysis. In: Handbook of Chemical Property Estimation Methods, Lyman W, Reehl W and Rosenblatt D (eds.), Chapter 8. McGraw-Hill Book Company, New York, USA.

Hine C, Anderson H and Kodama J (1955). Sensory thresholds of certain Shell organic solvents, Progress Report 1, Report to Shell Development Company, November 15, 1955, UC Report #247.

Kimura E, Ebert D and Doge P (1971). Acute toxicity and limits of solvent residues for sixteen organic solvents. Toxicol. Appl. Pharmacol. 19:699-704.

Harris J (1982b). Rate of hydrolysis. In: Handbook of Chemical Property Estimation Methods, Lyman W, Reehl W and Rosenblatt D (eds.), Chapter 7. McGraw-Hill Book Company, New York, USA.

IPCS (International Programme on Chemical Safety) (1993). Methyl Ethyl Ketone. Environmental Health Criteria 143. World Health Organization, Geneva, Switzerland.

Isoproanol Panel, American Chemistry Council (2006). Test Plan for Diisopropyl Ether (DIPE) CAS No. 108-20-3. American Chemistry Council, Isopropanol Panel, Diisopropyl Ether HPV Task Group, Arlington, VA, USA.

Kamil I, Smith J and Williams R (1952). The metabolism of aliphatic alcohols. The glucuronic acid conjugation of acyclic aliphatic alcohols. Biochem. 53:129-136.

Kim, Y-H and K-H Engesser (2004). Degradation of Alkyl Ethers, Aralkyl Ethers, and Dibenzyl Ether by *Rhodococcus* sp. Strain DEE5151, Isolated from Diethyl Ether-Containing Enrichment Cultures. Applied and Environmental Microbiology Vol 70 (7), pp. 4398-4401.

Klimisch H, Andreae M and Tillmann U (1997). A systematic approach for evaluating the quality of experimental toxicological and ecotoxicological data. Regulatory Toxicol. Pharmacol. 25:1-5.

Liira J, Riihimäki V and Pfäffli P (1988). Kinetics of methyl ethyl ketone in man: Absorption, distribution and elimination in inhalation exposure. International Archives of Occupational Environ. Health. 60:195-200.

Lyon R, McComb J, Schreurs J and Goldstein D (1981). A relationship between alcohol intoxication and the disordering of brain membranes by a series of short-chain alcohols. J. Pharmacol. Exp. Ther. 218:669-675.

Machle W, Scott E and Treon J (1939). The physiological response to isopropyl ether and to a mixture of isopropyl ether and gasoline. J. Ind. Hyg. Toxicol. 21:72-96.

Mackay D, Di Guardo A, Paterson S and Cowan C (1996). Evaluating the environmental fate of a variety of types of chemicals using the EQC model. Environ. Toxicol. Chem. 15:1627-1637.

Mackay D, DiGuardo A, Paterson S and Cowan C (2003). EQC Model version 2.02, available from the Environmental Centre, Trent University, Canada

Marsh D and Leake C (1950). The Comparative Anesthetic Activity of the Aliphatic Ethers. Anesthesiology. 11(4): 455-463.

Mellon (Mellon Institute of Industrial Research) (1951). Project Report Number 14-78. Union Carbide Corporation, Danbury, CT, USA.

Mill T (2000). Photoreactions in surface waters. In: Handbook of Property Estimation Methods for Chemicals, Boethling R and Mackay D (eds.), Chapter 15. Lewis Publishers, New York, USA.

Munies R and Wurster D (1965). Investigation of some factors influencing Percutaneous absorption III: absorption of methyl ethyl ketone. J. Pharm. Sci. 54:1281-1284.

Neely W (1985). Hydrolysis. In: Environmental Exposure from Chemicals. Vol. 1. Neely W and Blau G (eds.), pp. 157-173. CRC Press, Boca Raton, FL, USA.

Nelson B, Brightwell W, Khan A, Burg J and Goad P (1989). Lack of selective developmental toxicity of three butanol isomers administered by inhalation to rats. Fundam. Appl. Toxicol. 12:469-479.

O'Donoghue J, Haworth S, Curren R, Kirby P, Lawlor T, Moran E, Phillips R, Putnam D, Rogers-Back A, Slesinski R and Thilagar A (1988). Mutagenicity studies on ketone solvents: methyl ethyl ketone, methyl isobutyl ketone, and isophorone. Mut. Res. 206:149-161.

Page D and Carlson G (1993). Effect of pyridine on the hepatic and pulmonary metabolism of 2-butanol in rat and rabbit. J. Toxicol. Environ. Health. 38:369-379.

Price J (1986). Toxicology of industrial chemicals (solvents): The acute oral and percutaneous toxicity, skin and eye irritancy and skin sensitizing potential of secondary butyl alcohol. Shell Research Report SBGR.86.108. Shell Research Limited, Sittingbourne Research Centre, Sittingbourne, England.

Rand M and Li C (1994). Effects of ethanol and other aliphatic alcohols on NO-mediated relaxations in rat anococcygeus muscles and gastric fundus strips. Br. J. Pharmacol. 111:1089-1094.

Rodriguez S and Dalbey W (1997). Subchronic neurotoxicity of vaporized diisopropyl ether in rats. International J. Toxicol. 16:599-610.

Saito (1975). The metabolism of lower alcohols. Nippon Ishi, 34:569-585 [Japanese; English translation].

Silverman L, Schulte F and First M (1946). Further studies on sensory response to certain industrial solvent vapors. J. Ind. Hyg. Toxicol. 28(6):262-266.

Smyth H, Carpenter C, Weil C and Pozzani U (1954). Range-finding toxicity data: List V. Arch. Ind. Hyg. Occup. Med. 10:61-68.

Snyder R and Andrews L (1996). Toxic effects of solvents and vapors. Chapter 24. In: Casarett & Doull's Toxicology. The Basic Science of Poisons. 5th Edition. Ed. C.D. Klaassen. McGraw-Hill, New York, NY, USA.

Tanii H, Zhang X and Ohyashiki T (1995). In vitro influences of alcohols on mouse synaptosomes, and structure-activity relationships. Arch. Toxicol. 69:617-623.

Traiger G, Bruckner J, Jiang W, Dietz F and Cooke P (1989). Effect of 2-butanol and 2-butanone on rat hepatic ultrastructure and microsomal drug metabolizing enzyme activity. J. Toxicol. Environ. Health. 28:235-248.

US EPA (1999a). Determining the Adequacy of Existing Data. OPPT, EPA, Washington, DC, USA.

US EPA (1999b). The Use of Structure-Activity Relationships (SAR) in the High Production Volume Chemicals Challenge Program. OPPT, EPA, Washington, DC, USA.

Wallgren H (1960). Relative Intoxicating effects on rats of ethyl, propyl and butyl alcohols. Acta Pharmacol. Toxicol. 16:217-222.

Wass U and Belin L (1990). An *in vitro* method for predicting sensitizing properties of inhaled chemicals. Scand. J. Work Environ. Health. 116:208-214.

Williams R (1959). Detoxication Mechanisms, 2nd ed. pp. 66-67. Chapman and Hall, London, England.

Yashuda Y, Cabral A and Antonio A (1976). Inhibitory action of aliphatic alcohols on smooth muscle contraction. Pharmacol. 14:473-478.

Zepp R and Cline D (1977). Rates of direct photolysis in the aqueous environment. Environ. Sci. Technol. 11:359.366.

APPENDIX A: RELIABILITY CRITERIA

Adapted from Klimisch *et al.* (1997)

Code of Reliability (CoR)	Category of Reliability
1	Reliable without restriction
1a	GLP guideline study (OECD, EC, EPA, FDA, etc...)
1b	Comparable to guideline study
1c	Test procedure in accordance with national standard methods (AFNOR, DIN, etc...)
1d	Test procedure in accordance with generally accepted scientific standards and described in sufficient detail
2	Reliable with restrictions
2a	Guideline study without detailed documentation
2b	Guideline study with acceptable restrictions
2c	Comparable to guideline study with acceptable restrictions
2d	Test procedure in accordance with national standard methods with acceptable restrictions
2e	Study well documented, meets generally accepted scientific principles, acceptable for assessment
2f	Accepted calculation method
2g	Data from handbook or collection of data
3	Not reliable
3a	Documentation insufficient for assessment
3b	Significant methodological deficiencies
3c	Unsuitable test system
4	Not assignable
4a	Abstract
4b	Secondary literature
4c	Original reference not yet available
4d	Original reference not translated (e.g. Russian)
4e	Documentation insufficient for assessment

201-16472B

IUCLID

Data Set

Existing Chemical	:	ID: 6863-58-7
CAS No.	:	6863-58-7
EINECS Name	:	2,2'-oxybisbutane
EC No.	:	229-961-6
Common name	:	sec-Butyl Ether
Molecular Formula	:	C8H18O

Producer related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	16.10.2006

Substance related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	16.10.2006
Status	:	
Memo	:	ExxonMobil Chemical Company - HPV
Printing date	:	14.11.2006
Revision date	:	
Date of last update	:	14.11.2006
Number of pages	:	31
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

IUPAC Name	:	Butane, 2,2'-oxybis-
Smiles Code	:	O(C(CC)C)C(CC)C
Molecular formula	:	C8H18O1
Molecular weight	:	130.23
Petrol class	:	

07.11.2006

Purity type	:	typical for marketed substance
Substance type	:	organic
Physical status	:	
Purity	:	
Colour	:	
Odour	:	

08.11.2006

bis (2-butyl) ether

07.11.2006

di-sec-Butyl Ether

07.11.2006

sec-Butyl Ether

07.11.2006

1.4 ADDITIVES

1.10 SOURCE OF EXPOSURE

Type of search : Internal and External
Chapters covered :
Date of search : 16.10.2006

Remark : Search covered all Physical Chemical Properties, Environmental Fate, Aquatic and Mammalian Toxicity endpoints related to the CAS number.

08.11.2006

Type of search : Internal and External
Chapters covered :
Date of search : 25.05.2005

Remark : Search covered all Physical Chemical Properties, Environmental Fate, Aquatic and Mammalian Toxicity endpoints related to the CAS number.

08.11.2006

Type of search : Internal and External
Chapters covered :
Date of search : 20.05.2005

Remark : Search covered all Physical Chemical Properties, Environmental Fate, Aquatic and Mammalian Toxicity endpoints related to the CAS number.

08.11.2006

Value	:	= -100 °C
Sublimation	:	
Method	:	other: measured
Year	:	
GLP	:	no data
Test substance	:	other TS: CAS No. 6863-58-7; sec-butyl ether
Test substance	:	CAS No. 6863-58-7; sec-butyl ether
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable. Value was provided by the experimental database of the EPIWIN program.
Flag	:	Critical study for SIDS endpoint

14.11.2006 (6)

Value	:	= -73 °C
Sublimation	:	
Method	:	other: calculated
Year	:	2003
GLP	:	no
Test substance	:	other TS: CAS No. 6863-58-7; sec-butyl ether
Method	:	Calculated values using MPBPWIN version 1.41, a subroutine of the computer program EPIWIN version 3.12
Test condition	:	Melting Point estimations performed by MPBPWIN are based on the average result of the calculation methods of K. Joback and Gold and Ogle. Joback's Method is described in Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds. The Gold and Ogle Method simply uses the formula Tm = 0.5839Tb, where Tm is the melting point in Kelvin and Tb is the boiling point in Kelvin.
Test substance	:	CAS No. 6863-58-7; sec-butyl ether
Reliability	:	(2) valid with restrictions The result is a calculated value based on the chemical structure and represents a potential melting point for the substance with the CAS number listed under test substance.

14.11.2006 (6)

Value	:	= 116 °C at 1013 hPa
Decomposition	:	
Method	:	other: calculated
Year	:	2003
GLP	:	no
Test substance	:	other TS: CAS No. 6863-58-7; sec-butyl ether
Test condition	:	Boiling point calculated by MPBPWIN subroutine, which is based on the method of S. Stein and R. Brown in "Estimation of Normal Boiling Points from Group Contributions". 1994. J. Chem. Inf. Comput. Sci. 34: 581-587.

Test substance	:	CAS No. 6863-58-7; sec-butyl ether
Reliability	:	(2) valid with restrictions The result is a calculated value based on the chemical structure and represents a potential boiling point for the substance with the CAS number listed under test substance.
Flag	:	Critical study for SIDS endpoint

14.11.2006 (6)

Type	:	
Value	:	= .759 g/cm³ at 25 °C
Method	:	other: measured
Year	:	1935
GLP	:	no data
Test substance	:	other TS: CAS No. 6863-58-7; sec-butyl ether
Test substance	:	CAS No. 6863-58-7; sec-butyl ether
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were reported in the peer-reviewed literature and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

14.11.2006 (3)

Value	:	= 21.7 hPa at 25 °C
Decomposition	:	
Method	:	other (measured)
Year	:	1994
GLP	:	no data
Test substance	:	other TS: CAS No. 6863-58-7; sec-butyl ether
Test substance	:	CAS No. 6863-58-7; sec-butyl ether
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed following acceptable test methods and therefore considered reliable. Value was provided by the experimental database of the EPIWIN program. Reference given in EPI Suite: Yaws, CL (1994B).
Flag	:	Critical study for SIDS endpoint

14.11.2006 (6)

Value	:	= 29.7 hPa at 25 °C
Decomposition	:	
Method	:	other (calculated)
Year	:	2003
GLP	:	no
Test substance	:	other TS: CAS No. 6863-58-7; sec-butyl ether
Method	:	Vapor pressure calculation by MPBPWIN ver. 1.40 using calculation method of Grain.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property

estimation.

Test substance	:	CAS No. 6863-58-7; sec-butyl ether
Reliability	:	(2) valid with restrictions The result is a calculated value based on the chemical structure and represents a potential vapor pressure for the substance with the CAS number listed under test substance.

14.11.2006 (6)

Partition coefficient	:	octanol-water
Log pow	:	= 3.35 at 25 °C
pH value	:	
Method	:	other (measured)
Year	:	1992
GLP	:	no data
Test substance	:	other TS: CAS No. 6863-58-7; sec-butyl ether
Test condition	:	Specific methods were not given in the document reporting the measured value. Measurements were performed at the Chemicals Inspection and Testing Institute of Japan.
Test substance	:	CAS No. 6863-58-7; sec-butyl ether
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed at a well respected testing facility and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

14.11.2006 (2)

Partition coefficient	:	octanol-water
Log pow	:	= 2.87 at 25 °C
pH value	:	
Method	:	other (calculated)
Year	:	2003
GLP	:	no
Test substance	:	other TS: CAS No. 6863-58-7; sec-butyl ether
Method	:	Calculated values using KOWWIN version 1.67, a subroutine of the computer program EPIWIN version 3.12
Test condition	:	Octanol / Water Partition Coefficient estimations performed by KOWWIN are based on an atom/fragment contribution method of W. Meylan and P. Howard in "Atom/fragment contribution method for estimating octanol-water partition coefficients". 1995. J. Pharm. Sci. 84:83-92.
Test substance	:	CAS No. 6863-58-7; sec-butyl ether
Reliability	:	(2) valid with restrictions The result is a calculated value based on the chemical structure and represents a potential partition coefficient for the substance with the CAS number listed under test substance.

14.11.2006 (6)

Solubility in	:	Water
Value	:	= 330 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	

pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: measured
Year	:	1992
GLP	:	no data
Test substance	:	other TS: CAS No. 6863-58-7; sec-butyl ether
Test condition	:	Specific methods were not given in the document reporting the measured value. Measurements were performed at the Chemicals Inspection and Testing Institute of Japan.
Test substance	:	CAS No. 6863-58-7; sec-butyl ether
Reliability	:	(2) valid with restrictions Although the original data were not retrieved and reviewed for quality, they were developed at a well respected testing facility and therefore considered reliable.
Flag	:	Critical study for SIDS endpoint

14.11.2006 (2)

Solubility in	:	Water
Value	:	= 327 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: calculated
Year	:	2003
GLP	:	no
Test substance	:	other TS: CAS No. 6863-58-7; sec-butyl ether
Method	:	Calculated values using WSKOWWIN version 1.41, a subroutine of the computer program EPIWIN version 3.12
Test condition	:	Water Solubility estimations performed by WSKOWWIN are based on a Kow correlation method described by W. Meylan, P. Howard and R. Boethling in "Improved method for estimating water solubility from octanol/water partition coefficient". Environ. Toxicol. Chem. 15:100-106. 1995.
Test substance	:	CAS No. 6863-58-7; sec-butyl ether
Reliability	:	(2) valid with restrictions The result is a calculated value based on the chemical structure and represents a potential water solubility for the substance with the CAS number listed under test substance.

14.11.2006 (6)

2.9 FLAMMABILITY

Type	:	water
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
Deg. product	:	
Method	:	other (calculated): Technical discussion
Year	:	2006
GLP	:	
Test substance	:	other TS: CAS No. 6863-58-7; sec-butyl ether

Result :

Photolysis as a Function of Molecular Structure

The direct photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation (Harris, 1982). The reaction process is initiated when light energy in a specific wavelength range elevates a molecule to an electronically excited state. However, the excited state is competitive with various deactivation processes that can result in the return of the molecule to a non excited state.

The absorption of light in the ultra violet (UV)-visible range, 110-750 nm, can result in the electronic excitation of an organic molecule. Light in this range contains energy of the same order of magnitude as covalent bond dissociation energies (Harris, 1982). Higher wavelengths (e.g. infrared) result only in vibrational and rotational transitions, which do not tend to produce structural changes to a molecule.

The stratospheric ozone layer prevents UV light of less than 290 nm from reaching the earth's surface. Therefore, only light at wavelengths between 290 and 750 nm can result in photochemical transformations in the environment (Harris, 1982). Although the absorption of UV light in the 290-750 nm range is necessary, it is not always sufficient for a chemical to undergo photochemical degradation. Energy may be re-emitted from an excited molecule by mechanisms other than chemical transformation, resulting in no change to the parent molecule.

A conservative approach to estimating a photochemical degradation rate is to assume that degradation will occur in proportion to the amount of light wavelengths >290 nm absorbed by the molecule (Zepp and Cline, 1977).

Saturated hydrocarbons and R-OH groups do not absorb light above 290 nm (Harris J, 1982a). Therefore, these moieties are stable in regard to direct photolytic processes. Ethers are also stable as this group absorbs UV light in the far UV region, below 220 nm (Mill T, 2000), therefore, direct photolysis will not be an important transformation process for the degradation of sec-butyl ether in the environment.

References:

Harris, J. C. 1982. "Rate of Aqueous Photolysis," Chapter 8 in: W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, USA.

Zepp, R. G. and D. M. Cline. 1977. Rates of Direct Photolysis in the Aqueous Environment, Environ. Sci. Technol., 11:359-366.

Boethling, R.S., Mackay, D. 2000. Handbook of Property Estimation

Methods for Chemicals, CRC Press, Boca Raton, FL, USA.

Test substance : CAS No. 6863-58-7; sec-butyl ether
Flag : Critical study for SIDS endpoint
14.11.2006 (5)

Type : air
Light source : Sun light
Light spectrum : nm
Relative intensity : based on intensity of sunlight
INDIRECT PHOTOLYSIS
Sensitizer : OH
Conc. of sensitizer : 1500000 molecule/cm³
Rate constant : = .000000000000320784 cm³/(molecule*sec)
Degradation : % after
Deg. product :
Method : other (calculated): Calculated values using AOPWIN version 1.91, a subroutine of the computer program EPIWIN version 3.12
Year : 2003
GLP : no
Test substance : other TS: CAS No. 6863-58-7; sec-butyl ether

Result : Atmospheric Oxidation Potential

In the environment, organic chemicals emitted into the troposphere are degraded by several important transformation processes. The dominant transformation process for most compounds is the daylight reaction with hydroxyl (OH-) radicals (Atkinson, 1988, 1989). The rate at which an organic compound reacts with OH- radicals is a direct measure of its atmospheric persistence (Meylan and Howard, 1993).

AOPWIN estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. The rate constants estimated by the program are then used to calculate atmospheric half-lives for organic compounds based upon average atmospheric concentrations of hydroxyl radicals.

Since the reactions only take place in the presence of sunlight, the atmospheric half-lives are normalized for a 12-hour day.

Calculated* half-life (days)	OH- Rate Constant (cm3/molecule-sec)
0.333	32.0784 E-12

References:

Atkinson, R. 1988. Estimation of gas-phase hydroxyl radical rate constants for organic chemicals. Environ. Toxicol. Chem. 7:435-442.

Atkinson, R. 1989. Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds. J. Phys. Chem. Ref. Data Monograph No. 1, Amer. Inst. Physics & Amer. Chem. Soc., NY.

Meylan, W.M. and P.H. Howard. 1993. Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. Chemosphere 12:2293-2299.

Test condition :

Indirect photodegradation, or atmospheric oxidation potential, is based on the structure-activity relationship methods developed by R. Atkinson.

Temperature: 25°C
Sensitizer: OH radical
Concentration of Sensitizer: 1.5 E6 OH radicals/cm3

Test substance : CAS No. 6863-58-7; sec-butyl ether
Reliability : (2) valid with restrictions
The results include calculated data based on chemical structure as modeled by AOPWIN. The data represent a potential atmospheric half-life range for the test substance.
Flag : Critical study for SIDS endpoint
14.11.2006 (6)

Type : abiotic
t1/2 pH4 : at °C
t1/2 pH7 : at °C
t1/2 pH9 : at °C
Deg. product :
Method : other: technical discussion
Year : 2006
GLP :
Test substance : other TS: CAS No. 6863-58-7; sec-butyl ether

Result : Hydrolysis as a Function of Molecular Structure

Hydrolysis of an organic molecule occurs when a molecule (R-X) reacts with water (H2O) to form a new carbon-oxygen bond after the carbon-X bond is cleaved (Gould, 1959; Harris, 1982). Mechanistically, this reaction is referred to as a nucleophilic substitution reaction, where X is the leaving group being replaced by the incoming nucleophilic oxygen from the water molecule.

Chemicals that are susecptible to hydrolysis contain functional groups that can be displaced by a nucleophilic substitution reaction. Substances that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (Neely, 1985). The lack of a suitable leaving group renders a compound resistant to hydrolysis.

Sec-butyl ether is expected to be resistant to hydrolysis because it lacks a functional group that is hydrolytically reactive (Harris, 1982b). Therefore, hydrolysis will not contribute to its removal from the environment.

References:

Gould, E.S. (1959), Mechanism and Structure in Organic Chemistry, Holt, Reinhart and Winston, New York, NY, USA.

Harris, J.C. (1982), "Rate of Hydrolysis," Chapter 7 in: W.J. Lyman, W.F. Reehl, and D.H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, NY, USA.

Neely, W. B. 1985. Hydrolysis. In: W. B. Neely and G. E. Blau, eds. Environmental Exposure from Chemicals. Vol I., pp. 157-173. CRC Press, Boca Raton, FL, USA.

Test substance : CAS No. 6863-58-7; sec-butyl ether
Flag : Critical study for SIDS endpoint
14.11.2006 (4)

3.1.3 STABILITY IN SOIL

Type	:	fugacity model level III
Media	:	other: air - sediment(s) - soil - water
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)
Soil	:	% (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)
Soil	:	% (Fugacity Model Level II/III)
Method	:	other: Calculation according Mackay, Level III
Year	:	2006

Method :

The EQC Level III model is a steady state model that is useful for determining how the medium of release affects environmental fate. Level III fugacity allows non-equilibrium conditions to exist between connected media as steady state, and illustrate important transport and transformation processes.

Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.12 program. Measured input values were also used where available and obtained from the EPIWIN database or other reliable sources. Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, and sediment).

Input values used:
Molecular mass = 130.23 g/mol
Water solubility = 327 mg/L
Vapour pressure = 2170 Pa
log Kow = 2.87
Melting point = -100 deg C

Degradation half-lives:

Air - 4.0 hrs
Water - 360 hrs
Soil - 7200 hrs
Sediment - 72000 hrs

This model was run assuming the default emissions.

Result :

Air - 3.2%
Water - 44.8%
Soil - 51.1%
Sediment - 0.9%

Test substance	:	CAS No. 6863-58-7; sec-butyl ether
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

14.11.2006 (8)

Type	:	fugacity model level I
Media	:	other: air - biota - sediment(s) - soil - water
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)
Soil	:	% (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)
Soil	:	% (Fugacity Model Level II/III)
Method	:	other: Calculation according Mackay, Level I
Year	:	2006
Method	:	The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment. Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.12 program. Measured input values were also used where available and obtained from the EPIWIN database or other reliable sources. Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, and sediment). Input values used: Molecular mass = 130.23 g/mol Water solubility = 327 mg/L Vapour pressure = 2170 Pa log Kow = 2.87 Melting point = -100 deg C
Result	:	Air - 99.1% Water - 0.5% Soil - 0.4% Sediment - <0.01% Suspended Sed - <0.01% Biota - <0.01%
Test substance	:	CAS No. 6863-58-7; sec-butyl ether
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

14.11.2006 (8)

Type	:	aerobic
Inoculum	:	
Contact time	:	
Degradation	:	(±) % after
Result	:	other: not readily biodegradable
Deg. product	:	
Method	:	other: calculated using BIOWIN version 4.02
Year	:	2006
GLP	:	no

Test substance	:	other TS: CAS No. 6863-58-7; sec-butyl ether
Remark	:	Calculation of biodegradation and the timeframe for Primary and Ultimate biodegradation using BIOWIN version 4.02, a subroutine of the computer program EPI Suite version 3.12 as described by Howard, et al, 1994. BIOWIN contains six models (linear regression (BIOWIN 1), non-linear regression (BIOWIN 2), ultimate degradation to CO2 and H2O (BIOWIN 3), primary degradation (BIOWIN 4), linear regression estimate of the probability of passing the OECD 301C / MITI-1 ready biodegradation test (BIOWIN 5), and non-linear regression estimate of the probability of passing the OECD 301C / MITI-1 ready biodegradation test (BIOWIN 6). BIOWIN 1 - "Does Not Biodegrade Fast" BIOWIN 2 - "Does Not Biodegrade Fast" BIOWIN 3 - "Weeks" BIOWIN 4 - "Days-Weeks" BIOWIN 5 - "Does Not Biodegrade Fast" BIOWIN 6 - "Does Not Biodegrade Fast" According to the USEPA, BIOWIN 6 is better predictor of whether a chemical will pass or fail the OECD 301C / MITI-1 ready biodegradation test than BIOWIN 5.
Test substance	:	CAS No. 6863-58-7; sec-butyl ether
Reliability	:	(2) valid with restrictions The value was calculated based on the chemical structure as modeled by EPI Suite. This robust summary has a reliability rating of 2 because the data are modeled.
Flag	:	Critical study for SIDS endpoint
14.11.2006		(6) (7)

Type	:	aerobic
Inoculum	:	activated sludge
Concentration	:	100 mg/l related to Test substance related to
Contact time	:	
Degradation	:	= 3 - 4 (±) % after 28 day(s)
Result	:	other: not readily biodegradable
Deg. product	:	
Method	:	other: Japanese Guideline by MITI (1974). Comparable to OECD TG 301C, Modified MITI Test 1
Year	:	1992
GLP	:	no data
Test substance	:	other TS: CAS No. 6863-58-7; sec-butyl ether
Method	:	The test was conducted in accordance with "Biodegradation test of chemical substances by microorganisms etc". stipulated in the Order Prescribing the Items of the Test Relating to the New Chemical Substance (1974, Order of the Prime Minister, the Minister of Health and Welfare, the Minister of International Trade and Industry No 1). This guideline coresponds to "301C, Ready Biodegradability: Modified MITI Test 1" stipulated in the OECD Guidelines for Testing of Chemicals (1981).
Test condition	:	Sludge concentration = 30 mg/l
Test substance	:	Analogue substance CAS No. 142-96-1; n-butyl ether
Reliability	:	(2) valid with restrictions Although a standard method was not followed, the testing procedures followed generally accepted aerobic biodegradation guideline methods and although there was limited information on the specifics of the study, there was sufficient information on testing method and conditions in general to rate this study a 2.
14.11.2006		(2)

3.6 BOD5, COD OR BOD5/COD RATIO

Species	:	Cyprinus carpio (Fish, fresh water)
Exposure period	:	42 day(s) at °C
Concentration	:	
BCF	:	= 47 - 83
Elimination	:	
Method	:	other: guideline corresponds to OECD 305C, Degree of Bioconcentration in Fish (1981)
Year	:	
GLP	:	no data
Test substance	:	other TS: CAS No. 6863-58-7; sec-butyl ether
Result	:	At a concentration of 0.2 mg/L sec-butyl ether was shown to have bioconcentrate factor (BCF) range of 47 to 83, which is a log BCF range of 1.67 to 1.92. At a concentration of 0.02 mg/L sec-butyl ether was shown to have a BCF range of 30 to 114, which is a log BCF range of 1.48 to 2.06.
Test condition	:	Fish supplier was Sugishima fish farm, Kumamoto, Japan. Upon arrival, fish were placed in an acclimation tank with a flow through water system for 28 days at 25° +/-2° C. Test fish were then transferred to test tanks and reared again at the same temperature for approximately 1 month. At test initiation, average fish weight, length, and lipid content were, 30 g, 10 cm, and 2-5%, respectively. Fish were fed pelleted feed for carp supplied by Haigo Shiryo K.K.. Fish were fed approximately 2% of their total body weight daily. On days fish were sampled, they were not fed. The test systems included 100 L volume glass tanks with a flow ate of 200 to 800 ml/min at 25° +/-2° C. Dissolved oxygen was 6 to 8 mg/L. At test initiation there was a minimum of 15 fish per exposure level. Treatment levels were based on results of acute toxicity testing. Test water, test fish, and control fish were analyzed twice a week, every two weeks, and prior to test initiation as well as at termination, respectively. Recovery efficiency was determined in water and fish homogenate. Analytical results from the definitive studies were corrected based on efficiency results. Bioconcentration factors were calculated based on: test substance concentration in fish / test substance concentration in water. Two concentrations were evaluated: 0.2 mg/L and 0.02 mg/L.
Test substance	:	Analogue substance CAS No. 142-96-1; n-butyl ether
Reliability	:	(2) valid with restrictions Although a standard method was not followed, the testing procedures followed generally accepted fish bioconcentration guideline methods and although there was limited information on the specifics of the study, there was sufficient information on testing method and conditions in general to rate this study a 2.
Flag	:	Critical study for SIDS endpoint

14.11.2006 (2)

BCF	:	= 32.1
Elimination	:	

Method	:	other: calculated
Year	:	2006
GLP	:	no
Test substance	:	other TS: CAS No. 6863-58-7; sec-butyl ether
Method	:	Calculated values using BCFWIN version 2.15, a subroutine of the computer program EPIWIN version 3.12.
Test condition	:	BCFWIN estimates the bioconcentration factor (BCF) of an organic compound using the compound's log octanol-water partition coefficient (Kow). The estimation methodology used by BCFWIN is described in "Improved Method for Estimating Bioconcentration Factor (BCF) from Octanol-Water Partition Coefficient", SRC TR-97-006 (2nd Update), July 22, 1997. Log Kow used = 2.87 Estimated BCF = 32.1 Estimated Log BCF = 1.507
Test substance	:	CAS No. 6863-58-7; sec-butyl ether
Reliability	:	(2) valid with restrictions The result is a calculated value based on the chemical structure and represents a potential bioaccumulation factor for the substance with the CAS number listed under test substance.

14.11.2006 (6)

Type	:	other: calculated
Species	:	other: freshwater fish
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	= 14.7 calculated
Method	:	other: ECOSAR Computer Model
Year	:	2006
GLP	:	
Test substance	:	other TS: CAS No. 6863-58-7; sec-butyl ether
Test condition	:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPISuite computer model (2). 1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92. 2. EPI SuiteTM (2000). Estimation Program Interface Suite, version 3.12. Syracuse Research Corporation, Syracuse, NY, USA.
Test substance	:	CAS No. 6863-58-7; sec-butyl ether
Conclusion	:	Based on the calculated Kow value of 2.87, sec-Butyl Ether is expected to have an acute 96-hour LC50 of 14.7 mg/L and a Chronic Value of 2.2 mg/L
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

14.11.2006 (1)

Type	:	other: calculated
Species	:	other: freshwater fish
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	= 10.8 calculated
Method	:	other: ECOSAR Computer Model
Year	:	2006
GLP	:	no
Test substance	:	other TS: CAS No. 6863-58-7; sec-butyl ether
Test condition	:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPISuite computer model (2). 1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92. 2. EPI SuiteTM (2000). Estimation Program Interface Suite, version 3.12. Syracuse Research Corporation, Syracuse, NY, USA.
Test substance	:	Analogue substance CAS No. 142-96-1; n-butyl ether
Conclusion	:	Based on the calculated Kow value of 3.01, n-Butyl Ether is expected to have an acute 96-hour LC50 of 10.8 mg/L and a Chronic Value of 1.6

mg/L.

Reliability : (2) valid with restrictions
The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

14.11.2006 (1)

Type : semistatic
Species : Oryzias latipes (Fish, fresh water)
Exposure period : 48 hour(s)
Unit : mg/l
LC50 : = 30.7 measured/nominal
Limit test : no
Analytical monitoring :
Method : other: Japanese Industrial Standard (JIS K 0102-1986-71): Testing Methods for Industrial Wastewater.
Year : 1992
GLP : no data
Test substance : other TS: CAS No. 6863-58-7; sec-butyl ether

Test condition : Fish supplier was Nakashima fish farm, Kumamoto, Japan. Upon arrival, fish were placed in an acclimation tank with a flow-through water system for 3 to 5 weeks after external disinfection. The external disinfection was carried out under static conditions for about 24-hours in an acqueous solution containing 20 mg/l of Elbarju (Ueno Pharm. Co.) and 7 g/l sodium chloride.

Test fish were then placed in an acclimation tank with a flow-through system at 25°±2°C for about 28 days.

Dilution water for the test and culture was provided by a well of the Kurume Research Laboratories. Water temperature, pH, and dissolved oxygen were continuously monitored in the laboratory. Total hardness, evaporated residue, chemical oxygen demand, chloride ion, and other harmful substances were also monitored. The quality of the dilution water was confirmed to meet the standards of the Ministry of Health and Welfare in total hardness and evaporated residue. The other analyzed items met the water quality standards for fisheries.

Test tanks were round glass vessels with 4 liters of test water per level. The test was conducted at 25°±2°C. Ten fish were tested at each level for 48 hours under semi-static conditions (renewal of test water every 8 to 16 hours).

Test concentrations (levels) were not reported.

The 48-hour LC50 value was estimated by either the Doudoroff Method or the Probit Method.

Test substance : Analogue substance CAS No. 142-96-1; n-butyl ether
Reliability : (2) valid with restrictions
Although a standard method was not followed, the testing procedures followed generally accepted fish acute toxicity guideline methods and although there was limited information on the specifics of the study, there was sufficient information on testing method and conditions in general to rate this study a 2.

14.11.2006 (2)

Type :

Species	:	Daphnia sp. (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
EC50	:	= 16.7 calculated
Method	:	other: ECOSAR Computer Model
Year	:	2006
GLP	:	no
Test substance	:	other TS: CAS No. 6863-58-7; sec-butyl ether
Test condition	:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPISuite computer model (2). 1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92. 2. EPI SuiteTM (2000). Estimation Program Interface Suite, version 3.12. Syracuse Research Corporation, Syracuse, NY, USA.
Test substance	:	CAS No. 6863-58-7; sec-butyl ether
Conclusion	:	Based on the calculated Kow value of 2.87, sec-Butyl Ether is expected to have an acute 48-hour EC50 of 16.7 mg/L and a Chronic Value of 1.3 mg/L.
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

14.11.2006 (1)

Type	:	
Species	:	Daphnia sp. (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
EC50	:	= 12.5 calculated
Method	:	other: ECOSAR Computer Model
Year	:	2006
GLP	:	no
Test substance	:	other TS: CAS No. 6863-58-7; sec-butyl ether
Test condition	:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPISuite computer model (2). 1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92. 2. EPI SuiteTM (2000). Estimation Program Interface Suite, version 3.12. Syracuse Research Corporation, Syracuse, NY, USA.
Test substance	:	Analogue substance CAS No. 142-96-1; n-butyl ether
Conclusion	:	Based on the calculated Kow value of 3.01, n-Butyl Ether is expected to have an acute 48-hour EC50 of 12.5 mg/L and a Chronic Value of 1.0 mg/L.
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

14.11.2006 (1)

Species	:	other algae: green alga
Endpoint	:	
Exposure period	:	96 hour(s)
Unit	:	mg/l
EC50	:	= 11 calculated
Method	:	other: ECOSAR Computer Model
Year	:	2006
GLP	:	no
Test substance	:	other TS: CAS No. 6863-58-7; sec-butyl ether
Test condition	:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPISuite computer model (2). 1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92. 2. EPI SuiteTM (2000). Estimation Program Interface Suite, version 3.12. Syracuse Research Corporation, Syracuse, NY, USA.
Test substance	:	CAS No. 6863-58-7; sec-butyl ether
Conclusion	:	Based on the calculated Kow value of 2.87, sec-Butyl Ether is expected to have an acute 96-hour EC50 of 11.0 mg/L and a Chronic Value of 1.8 mg/L.
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

14.11.2006 (1)

Species	:	other algae: green alga
Endpoint	:	
Exposure period	:	96 hour(s)
Unit	:	mg/l
EC50	:	= 8.3 calculated
Method	:	other: ECOSAR Computer Model
Year	:	2006
GLP	:	no
Test substance	:	other TS: CAS No. 6863-58-7; sec-butyl ether
Test condition	:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPISuite computer model (2). 1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92. 2. EPI SuiteTM (2000). Estimation Program Interface Suite, version 3.12. Syracuse Research Corporation, Syracuse, NY, USA.
Test substance	:	Analogue substance CAS No. 142-96-1; n-butyl ether

Conclusion	:	Based on the calculated Kow value of 3.01, n-Butyl Ether is expected to have an acute 96-hour EC50 of 8.3 mg/L and a Chronic Value of 1.5 mg/L.
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

14.11.2006 (1)

Species	:	other: Freshwater Fish (calculated toxicity values are not species specific)
Endpoint	:	other: LC50
Exposure period	:	30 day(s)
Unit	:	mg/l
ChV	:	= 2.2 calculated
Method	:	other: ECOSAR Computer Model
Year	:	2006
GLP	:	no
Test substance	:	other TS: CAS No. 6863-58-7; sec-butyl ether
Test condition	:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPISuite computer model (2).

1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.

2. EPI SuiteTM (2000). Estimation Program Interface Suite, version 3.12. Syracuse Research Corporation, Syracuse, NY, USA.

Test substance	:	CAS No. 6863-58-7; sec-butyl ether
Conclusion	:	Based on the calculated Kow value of 2.87, sec-Butyl Ether is expected to have an acute 96-hour LC50 of 14.7 mg/L and a Chronic Value of 2.2 mg/L
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

14.11.2006 (1)

Species	:	other: Freshwater Fish (calculated toxicity values are not species specific)
Endpoint	:	other: LC50
Exposure period	:	30 day(s)
Unit	:	mg/l
ChV	:	= 1.6 calculated
Method	:	other: ECOSAR Computer Model
Year	:	2006
GLP	:	no
Test substance	:	other TS: CAS No. 6863-58-7; sec-butyl ether
Test condition	:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a

subroutine in the EPISuite computer model (2).

Test substance	:	Analogue substance CAS No. 142-96-1; n-butyl ether
Conclusion	:	Based on the calculated Kow value of 3.01, n-Butyl Ether is expected to have an acute 96-hour LC50 of 10.8 mg/L and a Chronic Value of 1.6 mg/L.
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

14.11.2006 (1)

Species	:	Daphnia sp. (Crustacea)
Endpoint	:	mortality
Exposure period	:	16 day(s)
Unit	:	mg/l
EC50	:	= 1.3 calculated
Method	:	other: ECOSAR Computer model
Year	:	2006
GLP	:	no
Test substance	:	other TS: CAS No. 6863-58-7; sec-butyl ether
Test condition	:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPISuite computer model (2).

1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.

2. EPI SuiteTM (2000). Estimation Program Interface Suite, version 3.12. Syracuse Research Corporation, Syracuse, NY, USA.

Test substance	:	CAS No. 6863-58-7; sec-butyl ether
Conclusion	:	Based on the calculated Kow value of 2.87, sec-Butyl Ether is expected to have an acute 48-hour EC50 of 16.7 mg/L and a Chronic Value of 1.3 mg/L.
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

14.11.2006 (1)

Species	:	Daphnia sp. (Crustacea)
Endpoint	:	mortality
Exposure period	:	16 day(s)
Unit	:	mg/l
EC50	:	= 1 - calculated
Method	:	other: ECOSAR Computer model
Year	:	2006
GLP	:	no
Test substance	:	other TS: CAS No. 6863-58-7; sec-butyl ether
Test condition	:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a

subroutine in the EPISuite computer model (2).

1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.

2. EPI SuiteTM (2000). Estimation Program Interface Suite, version 3.12. Syracuse Research Corporation, Syracuse, NY, USA.

Test substance : Analogue substance CAS No. 142-96-1; n-butyl ether

Conclusion : Based on the calculated Kow value of 3.01, n-Butyl Ether is expected to have an acute 48-hour EC50 of 12.5 mg/L and a Chronic Value of 1.0 mg/L.

Reliability : (2) valid with restrictions
The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

14.11.2006 (1)

5.11 ADDITIONAL REMARKS

(1) Cash G and Nabholz V (1999). ECOSAR Classes for Microsoft Windows, ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment Division. Washington, DC, USA.

(2) Chemicals Inspection and Testing Institute (CITI) (1992). Biodegradation and bioaccumulation data of existing chemicals based on the CSCL Japan. CITI (ed.). Chemical Products Safety Division, Basic Industries Bureau, Ministry of International Trade and Industry, Japan. Japan Chemical Industry Ecology-Toxicology and Information Center.

(3) Drake, Nathan L. (1935). Journal of the American Chemical Society. Vol 57, pp. 2623-2625 CAPLUS.

(4) EMBSI (2006) Hydrolysis: CAS No. 6863-58-7; sec-Butyl Ether.

(5) EMBSI (2006) Photodegradation (Direct): CAS No. 6863-58-7; sec-Butyl Ether.

(6) EPI SuiteTM (2000). Estimation Program Interface Suite, version 3.12. Syracuse Research Corporation, Syracuse, NY, USA.

(7) Howard, PH, Boethling, RS, Stitler, WM, Meylan, WM, Hueber, AE, Beauman, JA and Larosche, ME (1992). Predictive model for aerobic biodegradability developed from a file of evaluated biodegradation data. Environ Toxicol Chem 11, 593-603.

(8) Mackay D, DiGuardo A, Paterson S and Cowan C (2003). EQC Model ver. 2.02, available from the Environmental Centre, Trent University, Canada.

IUCLID

Data Set

Existing Chemical	:	ID: 108-20-3
CAS No.	:	108-20-3
EINECS Name	:	diisopropyl ether
EC No.	:	203-560-6
TSCA Name	:	Propane, 2,2'-oxybis-
Molecular Formula	:	C6H14O

Producer related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.05.2005

Substance related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.05.2005
Status	:	
Memo	:	HPV
Printing date	:	27.02.2006
Revision date	:	
Date of last update	:	27.02.2006
Number of pages	:	55
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type	**:**	
Substance type	**:**	organic
Physical status	**:**	liquid
Purity	**:**	
Colour	**:**	
Odour	**:**	

27.10.2005

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

2,2'-oxybis-propane

27.10.2005

2,2'-oxybispropane

27.10.2005

2-Isopropoxy Propane

27.10.2005

2-Isopropoxypropan

27.10.2005

2-isopropoxypropane

27.10.2005

Diisopropyl Ether

27.10.2005

Dipropyloxid

27.10.2005

IPE

27.10.2005

IPE; Diisopropylether; DIPE; 2-Isopropoxy propane

27.10.2005

Isopropyl Ether

27.10.2005

Isopropylether

27.10.2005

propane, 2,2'-oxybis-

27.10.2005

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value	:	= -86.8 °C
Sublimation	:	
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	other TS: Diisopropyl Ether (CAS # 108-20-3)
Test substance	:	CAS No. 108-20-3; diisopropyl ether; purity is unknown.
Reliability	:	(2) valid with restrictions The CRC Handbook of Chemistry and Physics is a peer reviewed publication. This robust summary has a reliability rating of 2 because there is insufficient information available on the method and analytical procedure.
Flag	:	Critical study for SIDS endpoint

07.12.2005 (25)

2.2 BOILING POINT

Value	:	= 68.5 °C at 1013 hPa
Decomposition	:	
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	other TS: Diisopropylether
Test substance	:	CAS No. 108-20-3; diisopropyl ether; purity is unknown.
Reliability	:	(2) valid with restrictions The CRC Handbook of Chemistry and Physics is a peer reviewed publication. This robust summary has a reliability rating of 2 because there is insufficient information available on the method and analytical procedure.
Flag	:	Critical study for SIDS endpoint

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2.3 DENSITY

Type	:	density
Value	:	= .7241 g/cm³ at 20 °C
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	other TS: Diisopropyl Ether (CAS # 108-20-3)
Test substance	:	CAS No. 108-20-3; diisopropyl ether; purity is unknown.
Reliability	:	(2) valid with restrictions The CRC Handbook of Chemistry and Physics is a peer reviewed publication. This robust summary has a reliability rating of 2 because there is insufficient information available on the method and analytical procedure.
Flag	:	Critical study for SIDS endpoint

07.12.2005 (25)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	= 198.65 hPa at 25 °C
Decomposition	:	
Method	:	
Year	:	
GLP	:	no data
Test substance	:	other TS: Diisopropyl Ether (CAS # 108-20-3)
Method	:	Method not specified.
Test substance	:	CAS No. 108-20-3; diisopropyl ether; purity is unknown.
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data were not reviewed for quality, however, the reference is from a peer-reviewed handbook.
Flag	:	Critical study for SIDS endpoint

07.12.2005 (9)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	= 1.52 at 25 °C
pH value	:	
Method	:	other (measured)
Year	:	
GLP	:	no data
Test substance	:	other TS: Diisopropylether
Method	:	Method not specified.
Test substance	:	CAS No. 108-20-3; diisopropyl ether; purity is unknown.
Reliability	:	(2) valid with restrictions The value cited by the authors is a measured and preferred value. This robust summary has a reliability rating of 2 because there is insufficient information available on the method and analytical procedure.
Flag	:	Critical study for SIDS endpoint

27.10.2005 (19)

Partition coefficient	:	octanol-water
Log pow	:	= 2.4 at °C
pH value	:	6.7
Method	:	other (calculated): Indirect method by reverse-phase HPLC
Year	:	
GLP	:	no
Test substance	:	other TS: diisopropyl ether (CAS No. 108-20-3)
Result	:	Log Pow = 2.4 (Pow = 250) at pH 6.7
Test condition	:	The HPLC system was a reverse-phase C18-coated silica gel column, 250 mm x 5 mm id, with a mobile phase of 3 volumes methanol and 1 volume water (final pH 6.7) at a flow rate of 1 mL/min. 100 mL samples of an approximate 1 mg/mL solution in the mobile phase were injected, and the emergence of the material was observed using refraction index detection. Thirty-one reference compounds were used to generate the linear relationship between log k (k = capacity factor) and log Pow. Using the HPLC retention time for the peak of the test substance, the log k was determined, and the log Pow value was calculated using the linear equation developed from the reference compounds. Log Pow was determined according to the following calculations: Retention time (RT), min = 5.7

Capacity factor, k = 0.87, k = (RTcmpd - RTunretained std)/RTunretained std
log k = -0.06
linear equation: log k = -0.930 + 0.357 log Pow

Reliability : (1) valid without restriction
12.12.2005 (11)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	= 8800 mg/l at 20 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	
Year	:	
GLP	:	no data
Test substance	:	other TS: Diisopropyl Ether (CAS # 108-20-3)

Test substance : CAS No. 108-20-3; diisopropyl ether; purity is unknown.
Reliability : (2) valid with restrictions
The Ullmann's Encyclopedia of Industrial Chemistry is a peer reviewed publication. This robust summary has a reliability rating of 2 because there is insufficient information available on the method and analytical procedure.
Flag : Critical study for SIDS endpoint
07.12.2005 (17)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
Conc. of substance	:	at 25 °C
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000 molecule/cm³
Rate constant	:	= .00000000002434 cm³/(molecule*sec)
Degradation	:	= 50 % after 5.3 hour(s)
Deg. product	:	
Method	:	other (calculated): Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.12
Year	:	
GLP	:	
Test substance	:	other TS: Diisopropyl Ether (CAS # 108-20-3)
Method	:	Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.12 Indirect photodegradation, or atmospheric oxidation potential, is based on the structure-activity relationship methods developed by R. Atkinson under the following conditions: Temperature: 25°C Sensitizer: OH- radical Concentration of Sensitizer: 1.5E6 OH- radicals/cm3
Remark	:	DIPE has the potential to volatilize to air, based on a vapor pressure of 19,865 Pa at 25°C (Daubert and Danner, 1989), where it is subject to atmospheric oxidation. In air, DIPE can react with photosensitized oxygen in the form of hydroxyl radicals (OH-). The computer program AOPWIN (atmospheric oxidation program for Microsoft Windows) (EPIWIN, 2000) calculates a chemical half-life for a 12-hour day (the 12-hour day half-life value normalizes degradation to a standard day light period during which hydroxyl radicals needed for degradation are generated), based on an OH-reaction rate constant and a defined OH- concentration. DIPE has a calculated half-life in air of 5.3 hours or 0.4 days (12-hour day), based on a rate constant of 24.34 E-12 cm3/molecule*sec and an OH-concentration of 1.5 E5 OH-/cm3.
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint
07.12.2005		(15)
Deg. product	:	
Method	:	
Year	:	
GLP	:	
Test substance	:	other TS: Diisopropyl Ether (CAS # 108-20-3)
Method	:	Technical discussion
Remark	:	Direct photochemical degradation occurs through the absorbance of solar radiation by a chemical substance in aqueous solution. If the absorbed energy is high enough, then the resultant excited state of the chemical may undergo a transformation. A prerequisite for direct photodegradation is the ability of one or more bonds within a chemical to absorb ultraviolet

(UV)/visible light in the 290 to 750 nm range. Light wavelengths longer than 750 nm do not contain sufficient energy to break chemical bonds, and wavelengths below 290 nm are shielded from the earth by the stratospheric ozone layer (Harris, 1982a).
An approach to assessing the potential for a substance to undergo photochemical degradation is to assume that degradation will occur in proportion to the amount of light wavelengths >290 nm absorbed by constituent molecules (Zepp and Cline, 1977). The oxygen non-bonding electrons in ethers do not give rise to absorption above 160 nm, which is why pure ether solvents can be used in spectroscopic studies. Consequently, DIPE is not subject to photolytic processes in the aqueous environment.

Reliability : (2) valid with restrictions
This robust summary has a reliability of 2 because it is a technical discussion and not a study.

Flag : Critical study for SIDS endpoint

07.12.2005 (46)

3.1.2 STABILITY IN WATER

Type : abiotic
t1/2 pH4 : at °C
t1/2 pH7 : at °C
t1/2 pH9 : at °C
Deg. product :
Method : other: Technical discussion
Year :
GLP : no data
Test substance : other TS: Diisopropyl Ether (CAS # 108-20-3)

Result : Hydrolysis of an organic chemical is the transformation process in which a water molecule or hydroxide ion reacts to form a new carbon-oxygen bond. Chemicals with leaving groups that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (Gould, 1959). The lack of a suitable leaving group renders a compound resistant to hydrolysis. DIPE is resistant to hydrolysis because it lacks a functional group that is hydrolytically reactive and Harris (1982b) identifies ether groups as generally resistant to hydrolysis. Therefore, hydrolysis will not contribute to the removal of diisopropyl ether from the environment.

Reliability : (2) valid with restrictions
This robust summary has a reliability of 2 because it is a technical discussion and not a study.

Flag : Critical study for SIDS endpoint

07.12.2005 (18) (20)

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	
Media	:	other: air - biota - sediment(s) - soil - water
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)
Soil	:	% (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)
Soil	:	% (Fugacity Model Level II/III)
Method	:	other: Calculation according Mackay, Level I
Year	:	
Remark	:	Physicochemical data used in the calculation: Parameter Value w/ Units Molecular Weight = 102.18 Temperature = 25° C Log Kow = 1.52 Water Solubility = 8,800 g/m3 Vapor Pressure = 19,865 Pa Melting Point = -86.8° C
Result	:	Using the Mackay Level I calculation, the following distribution is predicted for diisopropyl ether: %Distribution Compartment 97.83 Air 2.10 Water 0.06 Soil <0.01 Sediment <0.01 Suspended Sediment <0.01 Biota
Test substance	:	Diisopropyl Ether (CAS # 108-20-3)
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated.
Flag	:	Critical study for SIDS endpoint

07.12.2005 (28)

Type	:	fugacity model level III
Media	:	other
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)
Soil	:	% (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)
Soil	:	% (Fugacity Model Level II/III)
Method	:	other: Level III simulation using the Mackay Multimedia Environmental Model (Mackay, 2001)
Year	:	
Method	:	Level III simulation using the Mackay Multimedia Environmental Model (Mackay, 2001). Mass balances are calculated for the four bulk media of air (gas + aerosol), water (solution + suspended sediment + biota), soil, (solids + air + water), and sediment (solids + pore water). Equilibrium exists within, but not between media. Physical-chemical properties are used to quantify a chemical's behavior in an evaluative environment. Three types of chemicals are treated in this model: chemicals that partition into all media (Type 1), non volatile chemicals (Type 2), and chemicals with zero, or near-zero, solubility (Type 3). The model can not treat ionizing or speciating substances. The Level III model assumes a simple, evaluative environment with user-defined volumes and densities for the following homogeneous environmental media (or compartments): air, water, soil, sediment, suspended sediment, fish and aerosols.

This model provides a description of a chemical's fate including the important degradation and advection losses and the intermedia transport processes. The distribution of the chemical between media depends on how the chemical enters the system, e.g. to air, to water, or to both. This mode of entry also affects persistence or residence time.

The rates of intermedia transport are controlled by a series of 12 transport velocities. Reaction half-lives are requested for all 7 media. The advective residence time selected for air also applies to aerosols and the residence time for water applies to suspended sediment and fish. The advective residence time of aerosols, suspended sediment and fish cannot be specified independently of the air and water residence times.

Result : Output

	Mass%	Half life(hr)	Emissions(kg/hr)
Air	19.4	25.2	1000
Water	61.0	360	1000
Soil	19.5	720	1000
Sediment	0.1	3240	0

Test condition : Physchem Inputs
Molar Mass = 102.18
Data Temperature = 25 ºC
Water Solubility = 8800 mg/l exp.
Vapour Pressure = 19865 Pa exp.
Log Kow = 1.52 exp.
Melting Point = -86.8 ºC exp.

Reaction Half Lives in hours (if not available they can be predicted using EPIWIN)

Air (gaseous)	25.2
Water (no susp. part.)	360
Bulk Soil	720
Bulk Sediment	3240
Suspended Particles	360
Fish	360
Aerosol	25.2

Environmental Properties (EQC standard environment)
Dimensions (all defaults)
Densities (all defaults)
Organic carbon & Advection (all defaults)
Transport Velocities (all defaults)

Emission and Inflows (defaults used)
Air 1000 kg/hr
Water 1000 kg/hr
Soil 1000 kg/hr
Sediment 0 kg/hr

Test substance : Diisopropyl Ether, CAS No. 108-20-3

Conclusion : The majority of DIPE is calculated to partition into the water phase, with smaller but significant amounts into air and soil, based on the modeling parameters used in this calculation. DIPE is considered to be a Type 1 chemical with potential to partition into all environmental compartments.

Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated.

Flag : Critical study for SIDS endpoint

01.11.2005 (27) (29) (30) (31)

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic
Inoculum : activated sludge, domestic
Contact time : 28 day(s)
Degradation : (±) % after
Result : other: not readily biodegradable
Deg. product :
Method : OECD Guide-line 301 D "Ready Biodegradability: Closed Bottle Test"
Year : 1982
GLP : no
Test substance : other TS: Diisopropyl Ether (CAS No. 108-20-3)

Result : Test substance was not readily biodegradable. After 28 days, the test substance exhibited no measurable biodegradation. By day 5, >60% biodegradation of positive control was observed, which meets the guideline requirement. No excursions from the testing guideline were noted. The inhibition study showed that the test substance did not inhibit the biodegradability of the positive control substance, sodium benzoate.

Sample	% Degradation* Mean (day 28)	% Degradation (day 28)
Test Substance	0.0, 0.0	0.0
Na Benzoate	65.0, 73.0	69.0

* duplicate data

Mean oxygen concentrations (mg/L) of duplicate test systems:

Day 0
Mineral Salts Control = 8.85
Blank = 8.8
Na Benzoate = 8.95
Test Substance = 8.9 (single test system)
Test Substance + Na Benzoate = 8.9* (single test system)

Day 5
Mineral Salts Control = 9.0
Blank = 8.8
Na Benzoate = 5.7
Test Substance = 8..85
Test Substance + Na Benzoate = 5.8

Day 15
Mineral Salts Control = 8.75
Blank = 8.65
Na Benzoate = 4.9
Test Substance = 8.55
Test Substance + Na Benzoate = 4.9

Day 28
Mineral Salts Control = 8.65
Blank = 7.05
Na Benzoate = 3.6
Test Substance = 8.3
Test Substance + Na Benzoate = 4.15

Test condition : The inoculum source was the Sittingbourne Sewage works in Kent,

England, and was prepared according to methods described in the OECD 301D guideline. The test substance was added to the test medium by direct addition at a concentration of 3.0 mg/L. Test systems were incubated at 20 ± 1 °C and biodegradation was determined by measuring the oxygen concentration on days 5, 15, and 28. Each sampling of the test substance and control was conducted in duplicate. The theoretical oxygen demand was 2.82 mg O2 per mg test substance and a theoretical carbon dioxide (CO2) evolution of 2.59 mg CO2 per mg test substance. Sodium benzoate was used as the positive control.

The purity of the test substance was not supplied, but the infra-red spectrum of the test substance matched a published standard (density = 0.723 to 0.726 kg/L). The test substance was stored in the dark at ambient temperature. Nitrogen was blown over the surface of the material when the container was opened and exposed to air in order to minimize peroxide formation.

Conclusion : Diisopropyl ether is not readily biodegradable and it did not significantly inhibit the biodegradability of the test substance in an inhibition test.

Reliability : (1) valid without restriction

07.12.2005 (40)

Type :
Inoculum : other: sanitary waste treatment plant effluent
Contact time : 5 day(s)
Degradation : (±) % after
Result :
Deg. product :
Method : other: American Public Health Association; No. 219 5-Day BOD; Standard Dilution Method
Year : 1971
GLP : no
Test substance : other TS: diisopropyl ether (CAS No. 108-20-3)

Remark : Test type: Biological Oxygen Demand (BOD)

Result : 0.19 g O2/g test material at 20 ± 1°C
The theoretical oxygen demand (ThOD) of the test substance was 2.82. The percent ThOD in 5 days was 7%.

The article stated that the only deviation from the standard method was the addition of 0.5 mg/L allylthiourea to prevent nitrification.

Test condition : The article stated that the test method followed APHA Standard Method No. 219 (1971). The test was run at a temperature of 20 ± 1°C. 500-mL test solutions were seeded with a filtered 10-mL volume of the effluent from a biological sanitary waste treatment plant. The activity of the inoculum was check by including a treatment containing a mixture of glucose and glutamic acid. Test mixtures were stirred using a magnetic stirrer.

Conclusion : 5-day BOD = 0.19 g/g, representing 7% biodegradation of the test substance.

Reliability : (2) valid with restrictions
The article presented a brief description of the testing methods, but cited a reliable guideline method in use at the time of the study.

07.02.2006 (2)

Type : aerobic
Inoculum : activated sludge
Deg. product :
Method : other: (comparison study of three aerobic biodegradation methods)
Year : 1997
GLP : no
Test substance : other TS: diisopropyl ether (CAS No. 108-20-3)

Method : Comparison study of three aerobic biodegradation methods)

Continuous Biological Treatment:
(1) EPA Method 304B (EPA, 1994)
Batch Methods:
(2) Batch Oxygen addition (BOX) (Rajagopalan et al., 1998), and
(3) Serum Bottle Test (SBT) (Rajagopalan et al., 1998)

Remark : Exposure Period:
Method 304: 30 days
BOX: 0.5 to 2 hours
SBT: 0.5 to 2 hours

Result : The average percent removal of the test substance in the continuous activated sludge unit (EPA Method 304B) was 99.4%.

Three experimental trial runs with each of the three biodegradation methods yielded the following average first-order biodegradation rate constants (K1 = L/g Volatile Suspended Solids-h) for the test substance:

	K1 (L/g VSS-h)
304B	98
BOX	17.4
SBT	19.2

Test condition : A pilot-scale continuous activated sludge unit served as the source of biomass for kinetic rate constant comparisons of the three methods. The activated sludge was acclimated in the pilot unit by feeding a synthetic cocktail of eight volatile organic compounds during a 2-month equilibration period. Equilibration and testing was done at ambient temperature (22 to 24°C). The hydraulic retention time (HRT) was 7.7 hours and the solids retention time (SRT) was 33 days. Average organic removal efficiencies based on COD and TOC were 92 and 88%, respectively.

During the biodegradation testing using Method 304B, feed and effluent samples were collected in headspace-free VOA vials and stored at 4°C until analyzed. Samples were analyzed by purge-and-trap gas chromatography using a flame ionization detector. Triplicate biodegradation runs on the test compound were conducted with at least six influent and effluent samples taken at 1 HRT (approx. 8 hours) intervals.

The two batch biodegradation testing methods (BOX and SBT) used activated sludge biomass from the pilot-scale reactor. Biomass was diluted using effluent from the system to achieve range of 200 to 600 mg/L. The test compound was injected into the batch reactors and the concentration was monitored over time by collecting gas samples directly from the headspace using an automatic sampling pump and analyzing immediately using gas chromatography.

Conclusion : The authors indicated that K1 values >10 L/g VSS-h represent readily biodegradable organic compounds. Based on the results of this study, all three test methodologies showed the test substance to be effectively utilized by activated sludge microorganisms under aerobic conditions.

Reliability : (2) valid with restrictions
The publication presented a well-documented study based on ound scientific principles.

07.02.2006 (6) (34) (42)

Type : aerobic
Inoculum : other: Mixture (see remarks)
Contact time : 600 day(s)
Degradation : (±) % after
Result :
Deg. product :
Method : other: (continuous-flow bioreactors)
Year : 2001
GLP : no
Test substance : other TS: diisopropyl ether (CAS No. 108-20-3)

Remark	:	Inoculum consisted of a mixture of the following: 1) mixed liquor from the Metropolitan Sewer District (MSD), Cincinnati, OH, 2) mixed liquor from Shell Development Co., Houston, TX, and 3) aquifer material wash water from a MTBE-contaminated site in Port Hueneme, CA.
Result	:	The authors indicated that removal of DIPE was comparable to that achieved for MTBE, which was greater than 99.9%.
Test condition	:	Bioreactors (Autoclave Engineers, Erie, PA) were initially seeded with 2 L of mixed liquor from the MSD, 600 mL of mixed liquor from Shell Development Co., and 140 mL of aquifer wash water. Cultures were maintained on a total influent feed of 417 mg/L chemical oxygen demand (COD) divided as 50% methyl tert-butyl ether (MTBE) and 50% as diisopropyl ether (DIPE). Reactors were well mixed and controlled to a temperature of 20°C. To retain high biomass levels, a polyethylene porous pot was inserted into the reactor. The pots consisted of 0.45 cm thick filter-grade polyethylene (pore size = 20 mm), with an internal diameter of 19.1 cm and a height of 29.2 cm. Initially, a solids retention time of 18 days was maintained by wasting intentionally from the reactor. Subsequently (after about 120 days) intentional wasting ceased and only took place during sampling of the reactors. The combined influent flow rate was 2.37 L/d, with 80% of the total flow provided by a pH-adjustment solution, and 20% provided by an acidified nutrient solution. The pH-adjustment solutions contained deionized water, MTBE and DIPE fed by a syringe infusion pump, and an appropriate amount of 10N sodium hydroxide to maintain the pH between 7.4 and 8.0. The nutrient solution consisted of deionized water with essential salts and vitamins added to promote biological growth. Final nutrient concentrations inside the reactor were as follows: (NH4)2SO4, 93 mg/L; MgSO4, 69.6 mg/L; CaCl2o2H2O, 22.5 mg/L; K2HPO4, 6.9 mg/L; CuSO4oH2O, 0.08 mg/L; Na2MoO4o2H2O, 0.15 mg/L; MnSO4oH2O, 0.13 mg/L; ZnCl2, 0.23 mg/L; CoCl2o6H2O, 0.42 mg/L; and FeCl2o4H2O, 17.25 mg/L.. The hydraulic retention time was 4.2 days with a total reactor volume of 9.95 L and an enrichment culture volume of 6 L. Effluent from the reactors was monitored weekly for the presence of MTBE and DIPE using gas chromatography equipped with a flame ionization detector (FID) and a 60/80 Carbopack B5% Carbowax 20 M glass column. The pH of the system was measured daily, and COD and dissolved organic carbon (DOC) was measured weekly.
Conclusion	:	Diisopropyl ether can be effectively biodegraded in high biomass aerobic reactors.
Reliability	:	(2) valid with restrictions The report provided adequate details of the test conditions but reported only a text description of biodegradation results.

07.02.2006 (33)

Type	:	
Inoculum	:	other: soil and groundwater from a site previously exposed to methyl tert-butyl ether
Contact time	:	1 year
Degradation	:	(±) % after
Result	:	
Deg. product	:	
Method	:	other: (soil/water microcosm)
Year	:	1999
GLP	:	no
Test substance	:	other TS: diisopropyl ether (CAS No. 108-20-3)

Remark	:	Test type: soil/water microcosm
Result	:	No detectable biodegradation of the test substance occurred after one year of incubation.
Test condition	:	Soil and water from an aquifer with previous exposure to methyl tert-butyl ether (MTBE) was collected using a coring device and a pump. The material was brought to the laboratory where the sediment was thoroughly mixed. Groundwater was filtered through a 0.45 mm filter and sparged for 12 hours with sterile air to oxygenate the water and to remove background volatile chemicals. Analysis by gas chromatography indicated that concentrations of MTBE in the aqueous samples were <10 mg/L. Microcosms were constructed in amber 255-mL screw-top bottles sealed with TeflonÒ MininertÒ valves. Each bottle contained 150 g of wet sediment, 140 mL of sterile groundwater and 3000 mg/L of diisopropyl ether (DIPE). Treatments were constructed in triplicate with matching abiotic controls. Sediment used for the abiotic controls was autoclaved for one hour on each of three consecutive days. Additionally, 250 mg/L of mercuric chloride was added to ensure no biological activity. Microcosms were incubated in the dark at 16 °C. All samples were analyzed every 30 days by purge and trap gas chromatography and flame ionization detection to determine concentrations of the test substance. Test substance disappearance relative to abiotic controls was the principal indicator of biodegradation.
Conclusion	:	The test substance was not aerobically biodegraded by indigenous subsurface microflora.
Reliability	:	(2) valid with restrictions The testing method did not follow any specific regulatory guideline method, but the publication provided valuable information using sound scientific principles.

07.02.2006 (45)

Type	:	anaerobic
Inoculum	:	other: sediment and groundwater from an anoxic aquifer polluted by municipal landfill leachate
Contact time	:	252 day(s)
Degradation	:	(±) % after
Result	:	
Deg. product	:	
Method	:	other: (closed serum bottle test)
Year	:	1993
GLP	:	no
Test substance	:	other TS: diisopropyl ether (CAS No. 108-20-3)
Result	:	Biodegradation Rate (ppm C/day) = 0 Methane recovery (% theoretical) = 0
Test condition	:	Diisopropyl ether was tested for the ability of the compound to be completely biodegraded to methane in an aquifer slurry. Sediment and groundwater were collected from a methanogenic portion of a shallow anoxic aquifer polluted by municipal landfill leachate. Slurries were prepared by placing 50 g of sediment and 75 mL of groundwater in sterile 160-mL serum bottles. The bottles were sealed with Teflon-lined stoppers and incubated in the dark at room temperature. Diisopropyl ether was added to the incubation mixture to reach an initial substrate concentration of 50 ppm C. Pressure increases resulting from biogas formation (CH4 and CO2) were monitored with an automated pressure transducer system. The acclimation time was estimated as the amount of time where no significant pressure difference was measured between the substrate-amended treatment and un-amended controls. At the end of the incubation period, biodegradation was measured as the depletion of parent substrate and the formation of methane over background controls. Measurements were made using gas

chromatography equipped with a flame ionization detector. A 1.8 m x 0.32 cm 80/100 porapak Q column or a 0.2% Carbowax 1500 on Carbopack C column were used for headspace methane analyses and test substance determinations, respectively. Autoclaved controls were similarly assayed and were uniformly unable to exhibit methane formation or test substance disappearance. The amount of methane formed in aquifer incubations was compared to that theoretically expected based on the Buswell equation.

Conclusion : Diisopropyl ether was a persistent molecule that resisted anaerobic destruction. After 252 days, no evidence for the anaerobic biodegradability of diisopropyl ether was obtained.

Reliability : (2) valid with restrictions
The publication reported a well-documented study that meets basic scientific principles.

07.02.2006 (41)

Type : anaerobic
Inoculum : other: Sediment and surface or groundwater
Deg. product :
Method : other: unknown
Year : 1994
GLP : no
Test substance : other TS: diisopropyl ether (CAS No. 108-20-3)

Remark : Exposure period: 85, 180, or 244 days
Result : Biodegradation of diisopropyl ether with sulfate or nitrate available as electron acceptors:

	SO4 or NO3 Substrate Loss (%)	Amount Consumed (% Theoretical)	Rate (umol/SO4/day)
sulfate-reducing	0	0	0
nitrate-reducing	0	0	0

Biodegradation of diisopropyl ether under methanogenic conditions:

	Degradation Rate (ppm C/day)	Methane Recovery (% Expected)
Fuel-impacted river sediment	0	0
Industrial/sewage impacted creek sediment	0	6

Test condition : Several tests were carried out to determine the anaerobic biodegradation of the test substance. Three experiments were done to determine biodegradation under sulfate- and nitrate-reducing conditions and under methanogenic conditions. Sediment and surface water (or groundwater) from three sources were used as inoculum in separate experiments; (1) sediment/groundwater from a landfill leachate impacted aquifer, (2) sediment/surface water from a river historically impacted by oil storage and barge loading facilities, and (3) sediment/surface water from a creek impacted by industrial waste and domestic sewage sludge.

Slurries were prepared by placing 50 g of sediment and 75 mL of water into sterile 160-mL serum bottles. Water was amended with sodium sulfide (1 mM) and resazurin (0.0002%) to serve as reductant and redox indicator, respectively. The bottles were sealed with stoppers and the headspace above the slurries was adjusted to 80% N2:20%CO2 (1 atm). To the landfill leachate-impacted samples, either sodium sulfate (5mM) or sodium nitrate (8 mM) was added in order to assess potential test substance decay coupled with the consumption of these electrons (referred to as sulfate-reducing and nitrate-reducing incubations, respectively). The test substance was added to the slurries to give an initial concentration of 50 ppm C. The rates of methane production, sulfate reduction, and nitrate

depletion were monitored in slurries receiving the test substance and compared to test substance-free controls. All incubations were done in the dark at 24°C. The sulfate-reducing experiment was run for 244 days, the nitrate-reducing experiment was run for 85 days, and the methanogenic experiment was run for 180 days.

In the methanogenic incubations, increases in headspace pressure were routinely monitored. Parent compound depletion and formation of methane were confirmed by gas chromatography (GC). The net amount of sulfate and nitrate depletion over the controls was monitored by high pressure liquid chromatrography (HPLC).

Conclusion : Diisopropyl ether is not anaerobically degraded under nitrate- or sulfate-reducing conditions, and it is not anaerobically degraded under methanogenic conditions.

Reliability : (2) valid with restrictions
The publication reported a well-documented study that meets basic scientific principles.

24.02.2006 (32)

Type : aerobic
Inoculum : other: Gordonia terrae strain IFP 2001 (CNCM Registration No. CTP 1-1889); isolated from activated sludge taken at an urban waste water treatment plant
Contact time : 24 hour(s)
Degradation : (±) % after
Result :
Deg. product :
Method : other: (sealed flasks, shaken)
Year : 2000
GLP : no
Test substance : other TS: diisopropyl ether (CAS No. 108-20-3)

Result : Diisopropyl ether was degraded by 78% over the 24-hour incubation period.

Comparison of DIPE biodegradation to ETBE:

Test Substance	Degradation (%)
ETBE	100

The authors indicated concentrations of the test substance in the flasks were quantified by analytical means. The method was not described in the report, but was referenced in an earlier publication by the same workers.

Test condition : The capacity of ethyl t-butyl ether (ETBE)-induced resting cells of the inoculum to degrade diisopropyl ether was tested in sealed flasks. The article focused on biodegradation of ETBE, methyl t-butyl ether (MTBE) and t-amyl methyl ether (TAME), but was tested on other ethers including diisopropyl ether (DIPE).

G. terrae IFP 2001 was cultivated on ETBE-supplemented MM medium. After 24 hours incubation, bacteria were harvested by centrifugation (20,000 g for 20 minutes), washed twice in 100 mM Tris-HCl buffer at pH 7.0 and re-suspended in Tris-HCl. The test substance was added to 20-mL cell suspensions in 125-mL sealed flasks. Flasks were incubated for 24 hours at 30 °C with orbital shaking. Initial cell concentration was 0.5 g/L. The test substance was tested at 100 mg/L. Filtered samples were analyzed at 0-hour and 24-hours.

Conclusion : Diisopropyl ether was degraded by 78% within 24 hours.

Reliability : (2) valid with restrictions
Information on the analytical method was not provided in the report.

07.02.2006 (21)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

Species	:	other: see remark
Exposure period	:	at 25 °C
Concentration	:	
BCF	:	= 2.95
Elimination	:	
Method	:	other: calculation
Year	:	
GLP	:	no
Test substance	:	other TS: Diisopropyl Ether (CAS # 108-20-3)
Remark	:	A log bioconcentration factor (BCF) of 0.47 is calculated (BCF = 2.95). With respect to a log Kow = 1.52, which was used to calculate the BCF, diisopropyl ether in the aquatic environment is expected to have a low bioaccumulation potential.
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

12.12.2005 (14)

Species	:	other: see remark
Exposure period	:	at 25 °C
Concentration	:	
BCF	:	= 14.06
Elimination	:	
Method	:	other: calculation
Year	:	
GLP	:	no
Test substance	:	other TS: Diisopropyl Ether (CAS No. 108-20-3)
Remark	:	A log bioconcentration factor (BCF) of 1.15 is calculated (BCF = 14.06). With respect to a log Kow = 2.4, which was used to calculate the BCF, disiopropyl ether in the aquatic environment is expected to have a low bioaccumulation potential.
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated and not measured.

12.12.2005 (14)

3.8 ADDITIONAL REMARKS

Memo	:	Biodegradation of diisopropyl ether
Remark	:	The article reports on a U.S EPA and American Petroleum Institute workshop (February 1-3, 2000) on biodegradation of methyl tert-butyl ether (MTBE)-contaminated soils and groundwater. MTBE is one of a group of structurally similar compounds commonly called alkyl ether oxygenates (AEO) that are added to reformulated gasoline to reduce carbon monoxide and ozone emissions. Diisopropyl ether (DIPE) is one type of AEO that is used in gasoline along others in this class of chemicals. The workshop focused on the status of the current research and understanding on biodegradation of MTBE and reported relevant information on the biodegradation of DIPE and other AEOs used in reformulated gasoline.

Pure microbial cultures have been identified and isolated that have demonstrated the capability of utilizing MTBE as a sole carbon and energy source under aerobic conditions (Scow et al., 2000). This isolate, bacterial strain PM1, was studied by Church and Tratnyek (2000) to determine the aerobic degradation pathway of MTBE. In their study, the authors confirmed the mineralization of MTBE and determined the degradation rates of DIPE and other AEOs were of the same order of magnitude as the degradation rates of MTBE (Church and Tratnyek, 2000). Their results suggested that similar enzyme systems were responsible for all of the reactions.

While the majority of research on anaerobic biodegradation of these compounds has been unable to show that MTBE is utilized, a few studies have demonstrated that MTBE and other AEOs may be susceptible to attack under anaerobic conditions. Kropp et al. (2000) studied the anaerobic biodegradation potential of MTBE, DIPE, and other oxygenates in sediment slurries under methanogenic conditions. They found definite evidence in the form of methane and carbon dioxide production to conclude that anaerobic degradation was occurring. The workshop authors concluded that anaerobic biodegradation was a phenomena that was not widespread and extremely difficult for these compounds.

07.02.2006 (7) (12) (24) (36)

Memo : Biodegradation of diisopropyl ether under aerobic and anaerobic conditions - summary

Remark : Diisopropyl ether (DIPE) is one of a group of similar compounds referred to as alkyl ether oxygenates (AEO) that are added to reformulated gasoline. Biodegradation studies with DIPE and other AEO compounds have demonstrated the ability of these substances to be consumed by pure strains and mixed cultures of bacteria when incubated under aerobic conditions. Church and Tratnyek (2000) showed that bacterial strain PM1, which had been acclimated to methyl t-butyl ether (MTBE), could mineralize MTBE and demonstrated similar degradation rates for DIPE and other AEOs. They concluded that similar enzymes were responsible for all the degradation reactions. Additional evidence showing the wide spectrum of activity of the bacterial enzyme systems to degrade AEOs was provided by Hernandez-Perez et al. (2001). Using isolated Gordonia terrae (strain IFP 2001) that had been grown on ethyl t-butyl ether (ETBE), degradation of a variety of other AEOs could be achieved. DIPE was degraded 78% within 24 hours in their study (Hernandez-Perez et al. 2001).

Optimum biodegradation in mixed culture systems occurred when the microbial culture is allowed a period of acclimation to the substrate. For example, Bridié et al. (1979) measured only 7% consumption of the theoretical oxygen demand when DIPE was tested in a 5-day BOD test. In contrast, Cano et al. (1999) showed rapid utilization of DIPE when activated sludge was conditioned to a cocktail of volatile organic compounds for two months. In a continuous flow reactor, DIPE removal averaged 99.4%. Cano et al. (1999) also measured high rates of biodegradation of DIPE when comparing the continuous treatment method (EPA Method 304B) (EPA, 1994) to two batch treatment methods (BOX and SBT methods; Rajagopalan et al., 1998). Based on the measured rate constants, the authors considered DIPE to be readily biodegradable. Pruden et al. (2001) also observed high removal rates (e.g., 99.9%) of DIPE through a continuous flow reactor system. The performance of the reactors was enhanced when biomass was retained in the reactor, suggesting that a long biomass residence time may be needed for complete mineralization.

Biodegradation of DIPE is not always observed in biodegradation assays.

Zenker et al. (1999) failed to show biodegradation of DIPE over a 1-year period using indigenous microflora in sediment and water from an aquifer that had been previously exposed to MTBE. Given the apparent need of microbial communities for a period of acclimation to DIPE, it is unlikely that DIPE would be considered readily biodegradable in standard guideline studies. However, the evidence shows that DIPE can be inherently degraded by pure strains of bacteria and mixed enrichments of activated sludge microorganisms.

While available research shows that DIPE is capable of being biodegraded under aerobic conditions, anaerobic biodegradation is extremely difficult and this substance is considered recalcitrant under those conditions. Suflita et al. (1993) showed no biodegradation of DIPE after 252 days of anaerobic incubation. Substrate was added as 50 ppm C to sediment and groundwater collected from a methanogenic portion of a shallow anoxic aquifer. Similarly, DIPE was evaluated for anaerobic biodegradability under methanogenic conditions as well as sulfate and nitrate-reducing conditions (Mormile et al., 1994). Inocula from three sources (e.g., sediment/groundwater from an aquifer impacted by landfill leachate, sediment/surface water from a river impacted by oil storage, and sediment/surface water from a creek impacted by industrial waste and domestic sewage) were used in separate incubations to assess anaerobic biodegradation in sealed serum bottles. No DIPE biodegradation was measured over incubation periods of 85 days (nitrate-reducing conditions), 180 days (methanogenic conditions), and 244 days (sulfate-reducing conditions). Lack of methane production reported by Suflita and Mormile (1993) does not preclude partial anaerobic biodegradation of DIPE in their studies because only methane was monitored. Kropp et al. (2000) studied the anaerobic biodegradation potential of a number of AEOs including DIPE in sediment slurries under methanogenic conditions. They found evidence in the form of methane and carbon dioxide production to conclude that anaerobic biodegradation was occurring, although the authors stated that anaerobic biodegradation was not a widespread phenomena and extremely difficult for these compounds.

27.02.2006

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	flow through
Species	:	Pimephales promelas (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	= 91.7
Limit test	:	
Analytical monitoring	:	yes
Method	:	other: Flow-through Fish Acute Toxicity Test
Year	:	1983
GLP	:	no data
Test substance	:	other TS: Diisopropyl Ether (CAS No. 108-20-3)

Method :

The water solubility of the test chemical was obtained from literature or determined experimentally. A flow through system using proportional diluters and modified continuous mini-diluter system was used for maintaining the required test concentrations

Twenty to twenty-five 30 day-old fish, each weighing approximately 0.12 g, were randomly divided amongst the test tanks (control and five different concentrations) with flow-through dilutor systems.

Lake Superior water maintained at 25°C ± 1°C was used in the test. Routine measures of hardness (EDTA) and total alkalinity of test water yielded mean values of 45.5 and 42.2 mg/L as CaCO3, respectively. The arithmetic mean of the pH was 7.5 and dissolved oxygen was always greater than 60% of saturation.

Fish were supplied from the United States Environmental Protection Agency, Environmental Research Laboratory-Duluth culture. They were not fed during the test. Deaths were recorded after 1, 3, 6,12, 24, 48, 72, and 96 hours.

Remark : Statistics: Trimmed Spearman-Karber Method
Test method described in reference.

Result : 96-hour LL50 = 91.7 mg/L based upon measured values

Analytical method used was GC analysis with Flame Ionization Detection (GC-FID), performed on a Hewlett-Packard model 5730A gas chromatograph. Concentrations of the test chemical were measured daily at each exposure level.

Conclusion : 96-hour LC50 = 91.7 mg/L based upon measured values.

Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because complete information on the analytical results were not available and the study was not conducted under GLP.

Flag : Critical study for SIDS endpoint

01.11.2005 (43)

Type	:	
Species	:	other: Fish
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	= 214.1
Method	:	other: ECOSAR version 0.99h, US EPA
Year	:	
GLP	:	
Test substance	:	other TS: Diisopropyl Ether (CAS No. 108-20-3)

Method	:	ECOSAR version 0.99h, US EPA. The structure-activity relationships (SARs) presented in this program are used to predict the aquatic toxicity of chemicals based on their similarity of structure to chemicals for which the aquatic toxicity has been previously measured. Most SAR calculations in the ECOSAR Class Program are based upon the octanol/water partition coefficient (Kow). SARs have been used by the U.S. Environmental Protection Agency since 1981 to predict the aquatic toxicity of new industrial chemicals in the absence of test data. SARs are developed for chemical classes based on measured test data that have been submitted by industry or they are developed by other sources for chemicals with similar structures, e.g., phenols. Using the measured aquatic toxicity values and estimated Kow values, regression equations can be developed for a class of chemicals. Toxicity values for new chemicals may then be calculated by inserting the estimated Kow into the regression equation and correcting the resultant value for the molecular weight of the compound. To date, over 150 SARs have been developed for more than 50 chemical classes. These chemical classes range from the very large, e.g., neutral organics, to the very small, e.g., aromatic diazoniums. Some chemical classes have only one SAR, such as acid chlorides, for which only a fish 96-hour LC50 has been developed. The class with the greatest number of SARs is the neutral organics, which has SARs ranging from acute and chronic SARs for fish to a 14-day LC50 for earthworms in artificial soil. The ECOSAR Class Program is a computerized version of the ECOSAR analysis procedures as currently practiced by the Office of Pollution Prevention and Toxics (OPPT). It has been developed within the regulatory constraints of the Toxic Substances Control Act (TSCA). It is a pragmatic approach to SAR as opposed to a theoretical approach.
Result	:	LC50, 96 h, for fish = 214.1 mg/L
Test condition	:	Experimental water solubility, 8800 mg/l @ 20°C (Heitmann, W et al, 1987), log Kow, 1.52 (Funasaki, N et al, 1985) and melting point, -86.6°C (SRC PhysProp database) were entered into the program. Class: Neutral organics
Test substance	:	Diisopropyl Ether (CAS No. 108-20-3)
Conclusion	:	The predicted 96 h LC50 value for fish (214.1 mg/L) is in good agreement with the experimental 96 h LC50 value for fathead minnow (Pimephales promelas) (91.7 mg/L) (Veith et al., Can. J. Fish. Aquat. Sci., 40:743-748) and 48 h EC50 value for Daphnia (190.0 mg/L) (Stephenson R.R., Shell Research Limited, Report No. SBGR.83.215).
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated and not measured.

28.10.2005 (13)

Type	:	flow through
Species	:	Pimephales promelas (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	= 786
EC50	:	= 476
Limit test	:	
Analytical monitoring	:	yes
Method	:	other: Flow-through Fish Acute Toxicity Test
Year	:	1983
GLP	:	no data
Test substance	:	other TS: Diisopropyl Ether (CAS No. 108-20-3)

Method	:	Test solutions were prepared using a proportional diluter system without replication. This system provided control and five test substance concentrations to glass test vessels. Each vessel held 2 L of test solution and the diluter flow rate was sufficient to provide 18 volume additions per day. An aqueous stock solution of 1050 mg/L was used by the diluter to

prepare the exposure series. Dilution water was filtered Lake Superior water. Typical ranges of water quality factors measured in this water were pH (7.4 - 8.2), total hardness (44 - 53 mg/L as CaCO3), and specific conductance (78 - 86 mmhos/cm).

Test fish originated from in-house cultures of P. promelas at the U.S. EPA Environmental Research Laboratory - Duluth. Fish were not fed 24 h prior to testing or during the test. At test initiation, fish were randomly placed in test vessels until each vessel contained 10 individuals. Individuals used in testing were 34 d old and measured 19.0 mm mean length (SD = 2.534) and 0.104 g mean weight (SD = 0.0433). Biomass loading was 1.04 g/L. Death was the major test endpoint. Numbers of dead fish were counted daily and any dead fish were removed from the vessels. Abnormal behavioral changes were recorded at each observation time. LC50 (lethality) and EC50 (total effect) values were determined.

Temperature, dissolved oxygen, and pH were measured daily in all test chambers. Mean values (and Standard Deviation) were 24.9 °C (SD = 0.52), 7.3 mg/L (SD = 0.13), and 7.75 (SD = 0.16), respectively. Total hardness and alkalinity were measured once in the control, low, medium, and high test levels. Mean values were 43.7 mg/L total hardness as CaCO3 (SD = 0.96) and 49.6 mg/L alkalinity as CaCO3 (SD = 0.25). Lighting was provided by fluorescent bulbs that produced 28 to 48 lumens/sq ft at the water surface. The photoperiod was 16 h light and 8 h dark.

Test substance concentrations were verified in most cases daily during the test using gas-liquid chromatography. Concentrations were averaged and a mean percent recovery was calculated. The nominal with measured concentrations in parentheses were, control (not detected), 157 mg/L (131 mg/L), 242 mg/L (210 mg/L), 373 mg/L (382 mg/L), 574 mg/L (594 mg/L), and 883 mg/L (1044 mg/L). The overall percent recovery was 98.7%.

Remark : Statistics: LC/EC50 values determined by Trimmed Spearman-Karber Method

Result : 96-hour LC50 = 786 mg/L based on mean measured values.
96-hour EC50 = 476 mg/L based on mean measured values.

The EC50 value was based on mortality and the following abnormal effects: loss of schooling behavior, swimming near the surface, hypoactive, under-reactive to external stimuli, loss of equilibrium.

Conclusion : 96-hour LC50 = 786 mg/L based on mean measured values.
96-hour EC50 = 476 mg/L based on mean measured values.

Reliability : (1) valid without restriction
12.12.2005 (16)

Type : flow through
Species : Pimephales promelas (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
LC50 : = 900
Limit test :
Analytical monitoring : yes
Method : other: Flow-through Fish Acute Toxicity Test (ASTM, 1980)
Year : 1985
GLP : no data
Test substance : other TS: Diisopropyl Ether (CAS No. 108-20-3)

Method : Test solutions were prepared using a continuous-flow diluter delivery system, which delivered four test substance concentrations and control solutions to duplicate test vessels. Dilution water was filtered Lake Superior water. Average values for water quality factors for the dilution water were: hardness (44.6 mg/L as CaCO3), total alkalinity (44.0 mg/L as

CaCO3), and pH (7.6). Test chambers were glass vessels and contained 2 L of test solution. Solution flow rates through the test chambers was sufficient to provided at least a 95% replacement in approximately 4 h. Test substance concentrations were verified daily during the test using either gas chromatography or high pressure liquid chromatography methods.

The mean temperature for the test was 25 ± 0.5°C, and dissolved oxygen remained at or above 80% saturation. Lighting was provided by wide spectrum fluorescent bulbs at an intensity of 22 to 38 lumens/sq ft over the test chambers. The photoperiod was 16 h light and 8 h dark with a 30-min dusk/dawn transition period.

Test fish originated from cultures maintained by the U.S. EPA Environmental Research Laboratory - Duluth, MN. and were 28 to 34 days old (weighing approximately 0.12 g) at the time of testing. A total of 20 fish per treatment (10/replicate) was used in the test. Fish were added to the test chambers 2-3 h before introduction of the test solutions. Fish were not fed 24 h before or during the test. Mortalities were recorded daily.

Remark : Statistics: Trimmed Spearman-Karber Method or log-probit method.
Result : 96-h LC50 = 900 mg/L based on measured concentrations
95% CL = 881 - 920 mg/L
Conclusion : 96-h LC50 = 900 mg/L based on measured concentrations
Reliability : (1) valid without restriction
12.12.2005 (3)

Type : static
Species : Carassius auratus (Fish, fresh water)
Exposure period : 24 hour(s)
Unit : mg/l
LC50 : = 380
Limit test :
Analytical monitoring : yes
Method : other: static acute fish toxicity test (APHA, 1971)
Year :
GLP : no data
Test substance : other TS: Diisopropyl Ether (CAS No. 108-20-3)

Method : The test consisted of exposing groups of six fish to a series of concentrations of the test substance for 24 h. Fish were exposed in an all glass tanks holding 25 liters of test solution. Dilution water was local tap water having the following characteristics (all values in mg/L):
Cl^{-} = 65; $NO2^{-}$ = 0; $NO3^{-}$ = 4; $SO4^{-}2$ = 35; $PO4^{-}3$ = 0.15; $HCO3^{-}$ = 25; SiO2 = 25; NH4+ = 0; Fe = 0.05; Mn = 0; Ca+2 = 100; Mg+2 = 8; alkali as Na+ = 30; pH = 7.8.

The test was run at a temperature of 20±1°C, and the solutions were not aerated during the test period.

Test fish had a mean length of 6.2±0.7 cm, a mean weight of 3.3 ± 1.0 g and were in good health at the time of testing.

Exposure concentrations were confirmed either by total organic carbon analysis or by extraction and subsequent analysis by gas chromatography. Measured concentrations were not reported in this study.

Remark : Determination of LC50 by graphical interpolation of log concentrations versus percent mortality (APHA, 1971).
Result : 24-hour LC50 = 380 mg/L

The analytical method was either total organic carbon analysis or gas chromatography. It was not reported what method was employed for this test substance nor if the result was based on measured concentrations.

Conclusion	:	24-hour LC50 = 380 mg/L.
Reliability	:	(3) invalid The test was run for only 24 hours to ensure that the dissolved oxygen content did not fall below 4 mg/L. The report lacked sufficient detail for assessment. It was not stated whether results were based on nominal or measured values.

12.12.2005 (1)

Type	:	static
Species	:	Lepomis macrochirus (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	7000
Limit test	:	
Analytical monitoring	:	no
Method	:	other: static acute fish toxicity test
Year	:	
GLP	:	no
Test substance	:	other TS: Diisopropyl Ether (CAS No. 108-20-3)

Method :

The test consisted of exposing groups of fish to a four-dilution series of the test substance for a period of 96 h. Test vessels were all glass 5-gallon aquaria. The volume of test solution was adjusted to assure that a biomass loading was no more than 1 g fish /liter solution. Dilution water was well water having a typical pH of 7.6 to 7.9 and a hardness of 55 mg/L (as CaCO3).

Fish were obtained from a commercial source and assessed for health during a 14-d acclimation period prior to testing. During that time they were maintained on a commercial fish food diet supplemented with minced frozen shrimp. Fish were not fed 48 hours prior to testing. Fish were randomly selected for testing and were approximately 33 to 75 mm in length.

The test was run at 23°C. Test solutions were not aerated for the initial 24 h, but aeration was applied thereafter if the dissolved oxygen concentration was being depleted. Dissolved oxygen readings were taken daily, and pH was measured at the end of the test. However, these data were not provided in the report.

Mortality was assessed daily and any dead fish were removed at each observation time.

Remark	:	The LC50 was determined by plotting survival percentages on semi-logarithmic paper and drawing a straight line fit through or near significant points above and below 50% survival.
Result	:	96-hour LC50 = 7,000 mg/L

The mortality pattern reported for the test substance suggests that a more likely estimate of the LC50 value would lie between 7,900 and 10,000 mg/L, rather than 7,000 mg/L. This was due to a non-monotonic dose response pattern of mortality. The report authors indicated that the LC50 value was higher than the published solubility for the test substance.

Conclusion	:	96-hour LC50 = 7,000 mg/L based on nominal concentrations
Reliability	:	(3) invalid Documentation was insufficient for evaluation. Basic water quality data during the test were not provided. The authors stated that aeration of the test solutions was used after 24 hours to ensure maintenance of dissolved oxygen. No analytical verification of exposure concentrations were made.

12.12.2005 (10)

Type	:	static
Species	:	Menidia beryllina (Fish, estuary, marine)

Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	6600
Limit test	:	
Analytical monitoring	:	no
Method	:	other: static acute fish toxicity test
Year	:	
GLP	:	no
Test substance	:	other TS: Diisopropyl Ether (CAS No. 108-20-3)

Method :

The test consisted of exposing groups of fish to a four-dilution series of the test substance for a period of 96 h. Test vessels were all glass 5-gallon aquaria. The volume of test solution was adjusted to assure that a biomass loading was no more than 1 g fish /liter solution. Dilution water was prepared by adding "instant ocean" salts to well water (pH of 7.6 to 7.9; hardness 55 mg/L (as CaCO3)) until a specific gravity of 1.018 was achieved.

Fish were field collected in nets from Horseshoe Bay at Sandy Hook, New Jersey. They were held for a 14-d acclimation period prior to testing and assessed for health during that time. During the acclimation period they were fed minced frozen shrimp. Fish were not fed 48 hours prior to testing. Fish were randomly selected for testing and were approximately 40 to 100 mm in length.

The test was run at 20°C, and test solutions were continuously aerated during the exposure period. Dissolved oxygen readings were taken daily, and pH was measured at the end of the test. However, these data were not provided in the report.

Mortality was assessed daily and any dead fish were removed at each observation time.

Remark : LC50 determined by graphical interpolation of the logarithm of the concentration versus the percentage mortality.

Result : 96-hour LC50 = 6600 mg/L

The mortality pattern reported for the test substance does not correspond with the estimated LC50 value. Given the dose-response pattern, the LC50 value would lie between 3,200 and 5,000 mg/L, rather than 6,600 mg/L. The authors reported that the result was higher than the reported water solubility of the test substance.

Conclusion : 96-hour LC50 = 6600 mg/L based on nominal concentrations.

Reliability : (3) invalid
Documentation was insufficient for evaluation. Basic water quality data during the test were not provided. The authors stated that aeration of the test solutions was used after 24 hours to ensure maintenance of dissolved oxygen. No analytical verification of exposure concentrations were made.

12.12.2005 (10)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
EC50	:	= 190
Analytical monitoring	:	no
Method	:	other: U.S. Environmental Protection Agency, Methods for acute toxicity testing with fish, macro-invertebrates and amphibians (EPA-660/3-75-009)
Year	:	1975

GLP : no
Test substance : other TS: Diisopropyl Ether (CAS No. 108-20-3)

Remark : Statistics:
Probit analysis after log transformation of the concentrations (Finney, 1971)
Probit Analysis, Finney, D.J., Cambridge University Press, 3rd edition, p333 (1971)

Result : The 24 h and 48 h Effect Concentration (EC50) values were calculated to be 240 mg/L (95% fiducial limits 210 to 280 mg/L) and 190 mg/L (95% fiducial limits 160 to 220 mg/L), respectively.
The immobilization (%) of Daphnia magna (n=10/replicate) are as follows:

Test Substance Loading Rate (mg/L)	Immobilization (%)* 24 hr	48 hr
0 (control)	0	0
46	0	0
99	3	7
210	27	57
460	100	100
1000	100	100

*mean of 3 replicates

Test condition : A 48 hour static toxicity test was carried out without renewal of the test solutions. Quantities of stock solutions of di-isopropyl ether in acetone were added in triplicate sets of 110 mL glass flasks so that when made up with reconstituted freshwater, an approximately logarithmic series of concentrations ranging from 46 to 1000 mg/L was produced. Three flasks served as controls and received no test substance. The concentration of acetone in all control and test flasks was 0.1 mL/L. Precautions were taken to (a) minimise evaporative loss of the test substance by use of glass cover slips over the vessel necks and (b) to minimize the risk of organisms becoming trapped at the surface by placing black paper caps over the flasks to create a darkened zone which the organisms would avoid.
The test temperatures were in the range 20 ± 2°C, pH was in the range 8.2 to 8.4, the total hardness was 164 mg/L as CaCO3, and dissolved oxygen was in the range 8.2 to 9.2 mg/L.
The daphnids were cultured in-house, derived from a strain obtained (via ICI Brixham Laboratory) from Institut National de Recherche Chimique Applique (I.R.Ch.A.), France. Age was <24 hours old from 15 to 35 day old parents.
All concentrations of test substance are expressed in terms of quantities initially added to the test vessels.

Test substance : Diisopropyl Ether (CAS No. 108-20-3)
Conclusion : After Daphnia magna were exposed to test solutions of di-isopropyl ether for 48 hours in a static test, the 24 h and 48 h EC50 values were calculated to be 240 mg/L and 190 mg/L, respectively.
Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because it did not analytically verify exposure concentrations and the results are based on nominal values.

07.12.2005 (38)

Type :
Species : other: Daphnia
Exposure period : 48 hour(s)
Unit : mg/l
EC50 : = 221.9
Method : other: ECOSAR version 0.99h, US EPA
Year :
GLP :
Test substance : other TS: Diisopropyl Ether (CAS No. 108-20-3)

Method	:	ECOSAR version 0.99h, US EPA. The structure-activity relationships (SARs) presented in this program are used to predict the aquatic toxicity of chemicals based on their similarity of structure to chemicals for which the aquatic toxicity has been previously measured. Most SAR calculations in the ECOSAR Class Program are based upon the octanol/water partition coefficient (Kow). SARs have been used by the U.S. Environmental Protection Agency since 1981 to predict the aquatic toxicity of new industrial chemicals in the absence of test data. SARs are developed for chemical classes based on measured test data that have been submitted by industry or they are developed by other sources for chemicals with similar structures, e.g., phenols. Using the measured aquatic toxicity values and estimated Kow values, regression equations can be developed for a class of chemicals. Toxicity values for new chemicals may then be calculated by inserting the estimated Kow into the regression equation and correcting the resultant value for the molecular weight of the compound. To date, over 150 SARs have been developed for more than 50 chemical classes. These chemical classes range from the very large, e.g., neutral organics, to the very small, e.g., aromatic diazoniums. Some chemical classes have only one SAR, such as acid chlorides, for which only a fish 96-hour LC50 has been developed. The class with the greatest number of SARs is the neutral organics, which has SARs ranging from acute and chronic SARs for fish to a 14-day LC50 for earthworms in artificial soil. The ECOSAR Class Program is a computerized version of the ECOSAR analysis procedures as currently practiced by the Office of Pollution Prevention and Toxics (OPPT). It has been developed within the regulatory constraints of the Toxic Substances Control Act (TSCA). It is a pragmatic approach to SAR as opposed to a theoretical approach.
Result	:	EC50, 48 h, for Daphnia = 221.9 mg/L
Test condition	:	Experimental water solubility, 8800 mg/l @ 20°C (Heitmann, W et al, 1987), log Kow, 1.52 (Funasaki, N et al, 1985) and melting point, -86.6°C (SRC PhysProp database) were entered into the program. Class: Neutral organics
Test substance	:	Diisopropyl Ether, CAS No. 108-20-3
Conclusion	:	The predicted 48 h LC50 value for Daphnia (221.9 mg/L) is in close agreement with the experimental 48 h EC50 value for Daphnia (190.0 mg/L) (Stephenson R.R., Shell Research Limited, Report No. SBGR.83.215).
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated and not measured.

28.10.2005 (13)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	other algae: Green Alga
Endpoint	:	
Exposure period	:	96 hour(s)
Unit	:	mg/l
EC50	:	= 134.9
ChV	:	= 10.2
Method	:	other: ECOSAR version 0.99h, US EPA
Year	:	
GLP	:	
Test substance	:	other TS: Diisopropyl Ether (CAS No. 108-20-3)
Method	:	ECOSAR version 0.99h, US EPA. The structure-activity relationships (SARs) presented in this program are used to predict the aquatic toxicity of chemicals based on their similarity of structure to chemicals for which the

aquatic toxicity has been previously measured. Most SAR calculations in the ECOSAR Class Program are based upon the octanol/water partition coefficient (Kow). SARs have been used by the U.S. Environmental Protection Agency since 1981 to predict the aquatic toxicity of new industrial chemicals in the absence of test data. SARs are developed for chemical classes based on measured test data that have been submitted by industry or they are developed by other sources for chemicals with similar structures, e.g., phenols. Using the measured aquatic toxicity values and estimated Kow values, regression equations can be developed for a class of chemicals. Toxicity values for new chemicals may then be calculated by inserting the estimated Kow into the regression equation and correcting the resultant value for the molecular weight of the compound.

To date, over 150 SARs have been developed for more than 50 chemical classes. These chemical classes range from the very large, e.g., neutral organics, to the very small, e.g., aromatic diazoniums. Some chemical classes have only one SAR, such as acid chlorides, for which only a fish 96-hour LC50 has been developed. The class with the greatest number of SARs is the neutral organics, which has SARs ranging from acute and chronic SARs for fish to a 14-day LC50 for earthworms in artificial soil. The ECOSAR Class Program is a computerized version of the ECOSAR analysis procedures as currently practiced by the Office of Pollution Prevention and Toxics (OPPT). It has been developed within the regulatory constraints of the Toxic Substances Control Act (TSCA). It is a pragmatic approach to SAR as opposed to a theoretical approach.

Result : EC50, 96 h, for green algae = 134.9 mg/L

ChV, 96 h, for green algae = 10.2 mg/L

Test condition : Experimental water solubility, 8800 mg/l @ 20°C (Heitmann, W et al, 1987), log Kow, 1.52 (Funasaki, N et al, 1985) and melting point, -86.6°C (SRC PhysProp database) were entered into the program.
Class: Neutral organics

Test substance : Diisopropyl Ether (CAS No. 108-20-3)

Conclusion : The predicted 96 h EC50 value for algae (134.9 mg/L) is in the same range as the predicted 48 h LC50 value for Daphnia (221.9 mg/L) and the predicted 96 h LC50 value for fish (214.1 mg/L). There is also good comparison between the predicted and experimental EC50 values for Daphnia (221.9 mg/l v 190.0 mg/L, respectively) and for fish (214.1 mg/l v 91.7 mg/L, respectively).

Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated and not measured.

28.10.2005 (13)

Species : Selenastrum capricornutum (Algae)
Endpoint : biomass
Exposure period : 96 hour(s)
Unit : mg/l
EC50 : >= 1000
Limit test :
Analytical monitoring : no
Method : other: algae growth inhibition
Year : 1983
GLP : no data
Test substance : other TS: Diisopropyl Ether (CAS No. 108-20-3)

Method : A 4 d algal growth study was carried out using 10 concentrations of the test substance and a control. The test design included six control replicates and single vessels dosed with different concentrations of the test substance. 250-mL glass Erlenmeyer flasks served as the test vessels and held 50 mL of culture medium. Culture medium was prepare following the recipe given by Miller and Green (1978) with the following exceptions; 1)

boric acid concentration = 105 mg/L, and 2) sodium bicarbonate concentration = 50 mg/L.

To 10 flasks, quantities of a test substance stock solution made up in acetone were added to give a logarithmic series of concentrations ranging from 1 to 1000 mg/L (1.0, 2.2, 4.6, 10, 22, 46, 100, 220, 460, and 1000 mg/L). The concentration of acetone in all flasks including controls was adjusted to 0.1 mL/L. Each flask was inoculated with S. capricornutum to give an initial cell density of 5 x 102 cells/mL. The algal inoculum was prepared from an actively growing liquid culture of S. capricornutum in exponential growth phase.

Flasks were incubated in a temperature controlled orbital incubator under constant illumination (approximately 3000 lux) at 24±2°C for 4 days. Cell counts were made on days 2 and 4 using an electronic particle counter (Coulter counter). The temperature in the incubator was measured at 4-h intervals. The pH of the control and highest test concentration was measured on days 0, 2, and 4. Temperature remained within the 24±2°C specified range, and the pH ranged from 8.3 to 8.5 in the measured vessels.

All determination of EC50 values were based on nominal test concentrations and cell counts.

Result : 96-hour EC50 = >1000 mg/L based on nominal concentrations.

The 96-hour cell counts in the treated flasks as a percent of the mean control cell counts were:

1.0 mg/L = 84%	46 mg/L = 127%
2.2 mg/L = 108%	100 mg/L = 130%
4.6 mg/L = 91%	220 mg/L = 113%
10 mg/L = 122%	460 mg/L = 127%
22 mg/L = 129%	1000 mg/L = 91%

Conclusion : 96-hour EC50 = >1000 mg/L based on nominal concentrations.

Reliability : (3) invalid
Test concentrations were not measured and there is no indication in the report whether the test vessels were sealed. The reported LC50 value may reflect a loss of test substance by volatilization if the flasks were not tightly sealed.

12.12.2005 (39)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male/female
Number of animals	:	
Vehicle	:	other: None; administered undiluted
Doses	:	
Method	:	other: Similar to OECD 401
Year	:	
GLP	:	no
Test substance	:	other TS: Diisopropyl ether (CAS No. 108-20-3)
Method	:	Administered orally to nonfasted rats. LD50 calculated by the method of Litchfield and Wilcoxon [1949]. Similar to OECD 401.
Remark	:	Test type: Acute oral toxicity Year: Prior to 1971 No. of animals/dose: 6 male for young adult and older adult 6 - 12 male and female for 14-day old rats Route of administration: Oral gavage Dose level: Variable Dose volume: Variable Control group included: No, but none needed
Result	:	14-day old: LD50 6.4 ml/kg [approx 4.5 g/kg] young adults: LD50 16.5 ml/kg [approx 11.6 g/kg] Older adults: LD50 16.0 ml/kg [approx 11.2 g/kg] G/kg dose based on a density of 0.72 g/ml
Test condition	:	Rats were observed for up to 7 days after dosing.
Test substance	:	Diisopropyl ether (CAS No. 108-20-3) Chemical name: Isopropyl ether; isopropoxy propane, 2-; oxybis [propane], 2,2 '- Source/purity of test material is not specified, but stated to be analytical grade meeting ACS specifications.
Conclusion	:	DIPE, when administered to adult male Sprague-Dawley rats, had an acute oral LD50 of >10 g/kg. 14-day immature rats were considerable more sensitive [LD50 4.5 g/kg].
Reliability	:	(2) valid with restrictions Not GLP but conducted at a reputable laboratory [Abbot Laboratories, Chicago].

01.11.2005 (23)

Type	:	
Value	:	
Species	:	rabbit
Strain	:	New Zealand white
Sex	:	no data
Number of animals	:	6
Vehicle	:	other: none reported
Doses	:	8.2, 7.2, 6.0, 5.2, 3.3, 1.62 g/kg
Method	:	other: Similar to OECD 401
Year	:	
GLP	:	no

Test substance	:	other TS: Diisopropyl ether (CAS No. 108-20-3)
Remark	:	Test type: Acute oral toxicity Year: Prior to 1939 Route of administration: Oral Dose levels: 8.2, 7.2, 6.0, 5.2, 3.3, 1.62 g/kg Dose volume: Variable Control: No - none needed
Result	:	Minimal lethal dose between 7 - 9 ml/kg The symptoms noted were lack of coordination and unsteadiness at onset followed by a slight narcosis. In the animals that died the narcosis progressed towards a deep narcosis with loss of corneal reflex and evidences of depressant action on the medulla appeared, respiration became progressively slower, irregular and variable in amplitude and drop in body temperature till respiration failed. In the surviving animals, no effect on HB, erythrocyte count, total and differential leukocyte count was observed. No delayed toxicity was observed during the recovery period of 4 months after treatment.
Test substance	:	Diisopropyl ether (CAS No. 108-20-3) Chemical name: Isopropyl ether; isopropoxy propane, 2-; oxybis [propane], 2,2 '- Test material is stated to be commercial grade with 3% of isopropyl alcohol, but with no peroxide nor added inhibitor.
Conclusion	:	The test article, when administered orally as received to New Zealand white rabbits had a minimal lethal dose of 7 - 9 ml/kg [approx 5 - 6.5 g/kg].
Reliability	:	(2) valid with restrictions Not conducted by GLP but at a reputable laboratory [Kettering Laboratory, University of Cincinnati].

01.11.2005 (26)

5.1.2 ACUTE INHALATION TOXICITY

Type	:	
Value	:	
Species	:	guinea pig
Strain	:	other: not specified
Sex	:	no data
Number of animals	:	
Vehicle	:	other: none
Doses	:	0.3%; 1%; 3%; 6% in air
Exposure time	:	
Method	:	other: not specified
Year	:	
GLP	:	no
Test substance	:	other TS: Diisopropyl ether (CAS No. 108-20-3)
Remark	:	Test type: Acute inhalation toxicity Year: Prior to 1939 No. animlas/sex/group: One to two animals per dose Route of administration: Inhalation Dose level: 0.3%; 1%; 3%; 6% in air Dose volume: N/A Control: No
Result	:	0.3 % (~3000 ppm)- 2 h: No visible indication of anesthetic action 1 and 3.0 % (~30000 ppm)- 1 h: Not lethal; signs of anesthesia 6.0% (~60000 ppm) : Death as the result of respiratory failure within 1 hr
Test condition	:	1 or 2 hrs or until death [6%]
Test substance	:	Diisopropyl ether (CAS No. 108-20-3) Chemical name: Isopropyl ether; isopropoxy propane, 2-; oxybis [propane],

2,2 '-
Test material is stated to be commercial grade with 3% of isopropyl alcohol, but with no peroxide or added inhibitor.

Conclusion : The lowest lethal dose for 1 hr exposure was greater than 30,000 ppm in three species.

Reliability : (2) valid with restrictions
Not conducted by GLP. Few animals per group, but at a reputable laboratory [Kettering Laboratory, University of Cincinnati].

01.11.2005 (26)

Type :
Value :
Species : rabbit
Strain : New Zealand white
Sex : no data
Number of animals :
Vehicle : other: none
Doses : 0.3%; 1%; 3%; 6% in air
Exposure time :
Method : other: not specified
Year :
GLP : no
Test substance : other TS: Diisopropyl ether (CAS No. 108-20-3)

Remark : Test type: Acute inhalation toxicity
Year: Prior to 1939
No. animlas/sex/group: One to two animals per dose
Route of administration: Inhalation
Dose level: 0.3%; 1%; 3%; 6% in air
Dose volume: N/A
Control: No

Result : 0.3 % (~3000 ppm)- 2 h: No visible indication of anesthetic action
1 and 3.0 % (~30000 ppm)- 1 h: Not lethal; signs of anesthesia
6.0% (~60000 ppm) : Death as the result of respiratory failure within 1 hr

Test condition : 1 or 2 hrs or until death [6%]

Test substance : Diisopropyl ether (CAS No. 108-20-3)
Chemical name: Isopropyl ether; isopropoxy propane, 2-; oxybis [propane], 2,2 '-
Test material is stated to be commercial grade with 3% of isopropyl alcohol, but with no peroxide or added inhibitor.

Conclusion : The lowest lethal dose for 1 hr exposure was greater than 30,000 ppm in three species.

Reliability : (2) valid with restrictions
Not conducted by GLP. Few animals per group, but at a reputable laboratory [Kettering Laboratory, University of Cincinnati].

01.11.2005 (26)

Type :
Value :
Species : monkey
Strain : other: Macacus rhesus
Sex : female
Number of animals :
Vehicle : other: none
Doses : 0.3%; 1%; 3%; 6% in air
Exposure time :
Method : other: not specified
Year :
GLP : no
Test substance : other TS: Diisopropyl ether (CAS No. 108-20-3)

Remark : Test type: Acute inhalation toxicity

Year: Prior to 1939
No. animlas/sex/group: One to two animals per dose
Route of administration: Inhalation
Dose level: 0.3%; 1%; 3%; 6% in air
Dose volume: N/A
Control: No

Result : 0.3 % (~3000 ppm)- 2 h: No visible indication of anesthetic action
1 and 3.0 % (~30000 ppm)- 1 h: Not lethal; signs of anesthesia
6.0% (~60000 ppm) : Death as the result of respiratory failure within 1 hr

Test condition : 1 or 2 hrs or until death [6%]

Test substance : Diisopropyl ether (CAS No. 108-20-3)
Chemical name: Isopropyl ether; isopropoxy propane, 2-; oxybis [propane], 2,2 '-
Test material is stated to be commercial grade with 3% of isopropyl alcohol, but with no peroxide or added inhibitor.

Conclusion : The lowest lethal dose for 1 hr exposure was greater than 30,000 ppm in three species.

Reliability : (2) valid with restrictions
Not conducted by GLP. Few animals per group, but at a reputable laboratory [Kettering Laboratory, University of Cincinnati].

01.11.2005 (26)

5.1.3 ACUTE DERMAL TOXICITY

Type : LD50
Value :
Species : rabbit
Strain : New Zealand white
Sex : no data
Number of animals :
Vehicle : other: none
Doses : variable
Method : other: Similar to OECD 402
Year :
GLP : no
Test substance : other TS: Diisopropyl ether (CAS No. 108-20-3)

Remark : Test type: Acute dermal toxicity
Year: Prior to 1939
No. of animals/sex/group: Unspecified
Route of administration: Dermal
Dose level: variable
Control: No

Result : No deaths or systemic effects were reported. In rabbits dermal unoccluded LD50 > 2.0 g/kg. The actual dose applied was much higher, but continued to evaporate from the skin during application.

Test condition : The material was continuously dripped onto the shaved skin to keep it wet for one hour, while continuously evaporating. 150 ml of material was used.

Test substance : Diisopropyl ether (CAS No. 108-20-3)
Chemical Name: Isopropyl ether; isopropoxy propane, 2-; oxybis [propane], 2,2 '-
Test material is stated to be commercial grade with 3% of isopropyl alcohol, but with no peroxide or added inhibitor.

Conclusion : The test article, when administered dermally to New Zealand white rabbits had an acute dermal LD50 of greater than 2.0 g/kg.

Reliability : (2) valid with restrictions
Not GLP but conducted at a reputable laboratory [Kettering Laboratory, University of Cincinnati].

01.11.2005 (26)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

Type	:	other: In vitro chemical reactivity assay, surrogate for respiratory sensitization
Species	:	other: No animals; in vitro chemical assay
Number of animals	:	0
Vehicle	:	other: None
Result	:	not sensitizing
Classification	:	not sensitizing
Method	:	other: No guideline available
Year	:	1990
GLP	:	no
Test substance	:	other TS: Diisopropyl ether (CAS No.108-20-3)
Remark	:	Route of administration: N/A Sex: N/A Dose level: N/A Dose volume: N/A Control group included: Positive and negative controls included
Result	:	Diisopropanol was negative in this in vitro assay for potential respiratory sensitization. The assay gave positive responses with several known respiratory sensitizers.
Test condition	:	A method for monitoring chemical reactivity in aqueous solutions, at neutral pH and 37 degrees C, was developed. The chemical was allowed to react with a lysine-containing peptide, and the reaction was monitored with high-performance liquid chromatography. Simple acids, bases, and solvents did not react with the peptide, whereas isocyanates, anhydrides, and chloramine-T, substances well known for their sensitizing and asthma inducing properties, did. Thus a positive test strongly suggested that the chemical had the potential to act as a hapten and cause sensitization when inhaled.
Test substance	:	Diisopropyl ether (CAS No.108-20-3) Chemical Name: Isopropyl ether; isopropoxy propane, 2-; oxybis [propane], 2,2 '- Source/purity not specified.
Conclusion	:	Di-isopropanol was negative in this in vitro assay.
Reliability	:	(2) valid with restrictions Not conducted by GLP; research method not accepted by regulatory agencies; in vitro surrogate for respiratory sensitisation.

01.11.2005 (44)

5.4 REPEATED DOSE TOXICITY

Type	:	Sub-chronic
Species	:	rat
Sex	:	male/female
Strain	:	Sprague-Dawley
Route of admin.	:	inhalation

Exposure period	:	6 hours/day
Frequency of treatm.	:	5 days/week for ~13 weeks
Post exposure period	:	
Doses	:	0, 480, 3300, or 7100 ppm
Control group	:	other: yes (untreated & sham-exposed)
NOAEL	:	= 480 ppm
Method	:	EPA OTS 798.2450
Year	:	1996
GLP	:	no data
Test substance	:	other TS: Diisopropyl Ether (CAS No. 108-20-3)

Method : Statistical method:
Statistical analyses of numerical data included ANOVA and Tukey's studentized range test for data on serum chemistry. Duncan's multiple range test was used for hematology and body weights to assess statistically significant differences between control and exposed groups.

Remark : Male and female rats were acclimated for 2 weeks before initiation of exposures that began at ~8 weeks of age. Exposed animals were individually housed in 1-m3 inhalation chambers. Untreated control animals were housed in a separate room in identical caging. Room environment was set to 20-22ºC and 40-60% relative humidity. Lights were on a 12/12-hr light/dark cycle. Food and water were provided ad libitum except during exposures.

Vapors were generated by metering DIPE on to a warmed fiberglass wick and carried to the three 1m3 exposure chambers by a stream of measured and filtered room air. Temperature and humidity in the chambers were measured every 30 minutes and air flow through each chamber was metered to provide at least 12 air changes/hour. Chamber air samples were collected with a gas-tight syringe and analyzed with a gas chromatograph with a flame ionization detector and a fused silica column. Samples were periodically obtained for analysis by gas chromatography/ mass spectroscopy.

The primary endpoints during the course of exposures were individual body weights recorded weekly and clinical signs recorded daily except on weekends.

Following the last exposure, rats were fasted overnight and weighed; blood samples were obtained via the orbital sinus using light anesthesia. Samples were used to determine values for WBC, RBC, Hgb, Hct, MCV, MCH, MCHC, platelets, and differential counts. Glucose, urea nitrogen, total protein, albumin, globulin, A/G ratio, sorbitol dehydrogenase, aspartate aminotransferase, alanine aminotransferase, alkaline phosphatase, total bilirubin, creatinine, cholesterol, triglycerides, uric acid, Cl, Ca, Na, K, and P. Following the collection of blood samples, all animals were euthanized with sodium pentobarbital (i.p.) and exanguinated. Approximately 40 tissues were collected for histopathology and organs were weighed. Testis and associated tissues were preserved whole in 10% buffered formalin except for the left cauda epididymis of 10 rats in both control groups and the highest test group; epididymides were evaluated for morphology and number of sperm. The left testis in these groups was weighed and used for determination of number of testicular spermatids.

Type: 90-Day Subchronic
Species/strain: Rat/Sprague-Dawley; Tac:N(SD)fBR
No./sex/dose: 14/sex/group
Vehicle: None
Method: USEPA 1984, 40CFR Part 798:2450

Result : DIPE did not adversely affect clinical signs body weight, serum chemistry, hematology, or the number of sperm or spermatids. Exposure to males at

7100 ppm resulted in hypertrophy of liver cells associated with increased liver weight and in increased kidney weight with an increased incidence of hyaline droplets in proximal tubules of the kidney. Females had increased weight of both liver and kidney, although kidney increased only in relation to sham-exposed controls and no morphologic changes were observed in either organ. At 3300 ppm, weights of liver and kidney were increased in males; the liver weights were increased in females only compared to sham-exposed controls and not untreated controls. No morphologic abnormalities were observed. No changes were observed with 480 ppm.

Test substance : Diisopropyl Ether (CAS No. 108-20-3); purity ~92%.
Conclusion : NOAEL = 480 ppm
Reliability : (2) valid with restrictions
GLP unknown. Study well documented, meets generally accepted scientific principles, acceptable for assessment.

01.11.2005 (8)

Type : Sub-chronic
Species : rat
Sex : male/female
Strain : Sprague-Dawley
Route of admin. : inhalation
Exposure period : 6 hours/day
Frequency of treatm. : 5 days/week for ~13 weeks
Post exposure period :
Doses : 0, 450, 3250, or 7060 ppm
Control group : other: yes (sham-exposed)
Method : other: USEPA 1984, 40CFR Part 798:6050, 6400, and 6200
Year : 1997
GLP : no data
Test substance : other TS: Diisopropyl Ether (CAS No. 108-20-3)

Method : Statistical method:
All statistical analyses were performed with SAS software. Body weights, rectal temperatures fore- and hindlimb grip strengths, the number of rears, and motor activity were analyzed by a one-way analysis of variance followed by Duncan's multiple range test. The remaining data from the FOB were analyzed by Fisher's exact test using an extended contingency table containing all four groups of at given sex at a specified time. If a significant difference occurred for a given parameter, Fisher's exact test was used to directly compare each group individually against the control. Brain weights, lengths and widths, were analyzed by Student's t-test.

Remark : Male and female rats were acclimated for 2 weeks before initiation of exposures that began at ~8 weeks of age. Sham-exposed and exposed animals were individually housed in 1-m3 inhalation chambers except during behavioral testing, when they were placed in another room overnight and evaluated the following day. Room environment was set to 20-22ºC and 40-60% relative humidity. Lights were on a 12/12-hr light/dark cycle. Food and water were provided ad libitum except during exposures. Exposure vapors were generated by metering DIPE on to a warmed fiberglass wick and carried to the three 1-m3 exposure chambers by a stream of measured and filtered room air. Temperature and humidity in the chambers were measured every 30 minutes and air flow through each chamber was metered to provide at least 12 air changes/hour. Chamber air samples were collected with a gas-tight syringe and analyzed with a gas chromatograph with a flame ionization detector and a fused silica column. Samples were periodically obtained for analysis by gas chromatography/ mass spectroscopy.

Exposures were stagger-started over a 5-day period with 16 animals, 2/sex/group, receiving their first exposure on each of 5 consecutive days.

The rats were observed for signs of toxicity daily prior to initiation of

exposures, and individual body weights were recorded weekly.

During weeks of Functional Observation Battery (FOB) evaluation, four rats/group would be removed from the inhalation chamber and housed separately overnight and evaluated on the following day between the hours of 7:30 a.m. and 11:00 a.m. The process was repeated for each consecutive day until all rats were evaluated. The rats were evaluated with minimal disruption to the exposure schedule and with a manageable number of rats per day, 16 on any given day. The animals were evaluated in an FOB followed by a determination of motor activity prior to initiation of exposure; the FOB following 2, 4, 8, and 13 weeks of exposures, and for motor activity following 4, 8, and 13 weeks of exposures. Following the final determination of motor activity, the animals were anesthetized, intravascularly perfused, and the brain, spinal cord, and peripheral nerves removed for microscopic examination.

The FOB consisted of initially observing home-cage positioning, posture, and reaction to removal from the cage. This was followed by evaluation for exophthalmus/palpebral closure, lacrimation, salivation, pupillary response, palpebral reflex, and pinna reflex. These observations were scored by type and intensity. The animals were then observed for open field behavior. Piloerection, respiratory rate, tremors, convulsions, posture, gait, ataxic gait, tail elevation, unperturbed activity level, vocalization, number of rears, fecal balls, and urine pools were all recorded during the open-field observations. Reactions to the approach of a pencil, finger snap, and tail pinch were ranked and recorded. Finally, fore- and hindlimb grip strength , rectal temperature , and body weight were measured. Automated motor activity was assessed for 30 minutes in figure-eight mazes after the completion of the FOB.

Following the last FOB and motor activity evaluation, the rats were anesthetized with heparinized sodium pentobarbital (i.p.). The thoracic cavity was opened and the animals were infused with phosphate-buffered gluteraldehyde through the left ventricle. The perfused brain, spinal cord, and sciatic nerve with its tibial, sural, and peroneal divisions were removed. The brain and nerve tissues were processed for embedding in paraffin or glycol methacrylate (dorsal root ganglia and peripheral nerves) and sectioned for light or electron microscopic pathologic evaluation.

Type: 90-Day Neurotoxicity
Species/strain: Rat/Sprague-Dawley; Tac:N(SD)fBR
No./sex/dose: 10/sex/group
Vehicle: None
Method: USEPA 1984, 40CFR Part 798:6050, 6400, and 6200

Result : Motor activity in a figure-eight maze and unperturbed activity in the FOB were decreased at week 4 in females exposed to 7060 ppm; activity in the FOB was also decreased in females exposed to 450 ppm at week 4. Other changes in the FOB appeared to be minor, and no changes were observed during microscopic examination of tissues from the nervous system.

Test substance : Diisopropyl Ether (CAS No. 108-20-3); purity ~92%.

Conclusion : Inhalation exposures to DIPE at concentrations as high as 7060 ppm for 13 weeks resulted in few observable effects on the nervous system.

Reliability : (2) valid with restrictions
GLP unknown. Study well documented, meets generally accepted scientific principles, acceptable for assessment.

01.11.2005 (35)

5.5 GENETIC TOXICITY 'IN VITRO'

Type : Bacterial reverse mutation assay

System of testing	:	Salmonella typhimurium
Test concentration	:	Up to 8000 ug/ml in the pre-incubation mix
Cycotoxic concentr.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	other: Similar to OECD Guideline 471
Year	:	1988
GLP	:	no data
Test substance	:	other TS: Diisopropyl ether (CAS No. 108-20-3)

Remark :

Strains tested: Salmonella typhimurium tester strains TA98, TA100, TA1535, TA1537, TA1538

Exposure method: Preincubation assay for volatile compounds [Brooks and Dean 1981]

Test Substance Doses/concentration levels: Up to 8000 ug/ml in the pre-incubation mix

Metabolic activation: With and without (S9 fraction mix of livers of Aroclor 1254 pretreated rats)

Vehicle: Tween 80/ethanol

Tester strain, activation status, Positive Controls and concentration level: Not stated

Statistical analysis: Mean revertant colony count and standard deviation were determined for each dose point.

Dose Rangefinding Study: Cytotoxicity study

S9 Optimization Study: No

Result	:	DIPE did not induce reverse gene mutation in any strain. The test substance was not genotoxic in this assay with or without metabolic activation.
Test substance	:	Diisopropyl ether (CAS No. 108-20-3) Chemical Name: Isopropyl ether; isopropoxy propane, 2-; oxybis [propane], 2,2 '- Source/purity not specified.
Conclusion	:	Under the conditions of this study, the test material was not mutagenic.
Reliability	:	(2) valid with restrictions Restriction due to the lack of any information regarding the selection of dose levels used during the study. In addition no information is presented regarding cytotoxicity or the presence of test material precipitate in the cultures. Although study was not stated to be conducted under GLP, it was conducted at a reputable laboratory [Shell Research Limited, Sittingbourne Research Center].

10.11.2005 (5)

Type	:	Sister chromatid exchange assay
System of testing	:	Chinese hamster ovary cells
Test concentration	:	Up to 1200 ug/ml
Cycotoxic concentr.	:	
Metabolic activation	:	without
Result	:	negative
Method	:	other: Similar to OECD Guideline 473
Year	:	1984
GLP	:	no data
Test substance	:	other TS: Di-isopropyl ether (CAS No. 108-20-3)

Remark : Test type: Chromosome damage

Exposure method: For volatile compounds

Metabolic activation: Metabolic activation S9 was not added because liver cells are metabolically competent

Vehicle: Tween 80/ethanol

Tester strain, activation status, Positive Controls and concentration level: Cultured CHO cells were grown in 80 cm2 flasks for 24 hr before compound treatment. Treatment periods were 5 hr in the presence of S9 mix and 24 hr in the absence of S9. Colcemid was added to all cultures 22 hr after the initial treatment. After a further 2 hr, the cells were trypsinized, resuspended in hypotonic solution and then fixed, before spotting onto slides. Cell preparations were then stained with Giemsa. The slides were randomly coded and 100 cells from each culture were analyzed microscopically. Mitotic index estimations were also made. The positive controls were ethylmethanesulfonate [-S9] and cyclophosphamide [+S9].

Vehicle control: Yes

Dose rangefinding study: Cytotoxicity study

S9 Optimization study: No

Result : DIPE did not induce chromosomal damage in CHO cells. The test substance was not genotoxic in this assay.
Test substance : Di-isopropyl ether (CAS No. 108-20-3)
Chemical Name: Isopropyl ether; isopropoxy propane, 2-; oxybis [propane], 2,2 '-
Source/purity of test material: 98.5%
Conclusion : Under the conditions of this study, the test material was not mutagenic.
Reliability : (2) valid with restrictions
Restriction due to the lack of any information regarding the selection of dose levels used during the study. In addition no information is presented regarding cytotoxicity or the presence of test material precipitate in the cultures. Although study was not stated to be conducted under GLP, it was conducted at a reputable laboratory [Shell Research Limited, Sittingbourne Research Center].

10.11.2005 (4)

Type : DNA damage and repair assay
System of testing : Rat liver cells
Test concentration : Up to 1200 ug/ml
Cycotoxic concentr. :
Metabolic activation : without
Result : negative
Method : other: Similar to OECD Guideline 476
Year : 1984
GLP : no data
Test substance : other TS: Di-isopropyl ether (CAS No. 108-20-3)

Remark : Test type: Chromosome damage

Strains tested: RL4

Metabolic activation: Metabolic activation S9 was not added because liver cells are metabolically competent.

Vehicle: Tween 80/ethanol

Tester strain, activation status, Positive Controls and concentration level: Cultured rat liver cells were grown and treated on glass microscope slides

contained in 100 ml glass Leighton tubes. After 22 hr exposure to test compound or solvent, colcemid was added to each culture. After a further 2 hr, the slides were removed, subjected to hypotonic treatment followed by fixation and stained with Giemsa. The preparations were randomly coded and 100 cells from each culture were analyzed microscopically. The positive control was 7,12-dimethylbenzanthracenene.

Vehicle control: Yes

Dose rangefinding study: Cytotoxicity study

S9 Optimization study: None needed

Result : DIPE did not induce chromosomal damage in rat liver cells. The test substance was not genotoxic in this assay.
Test substance : Di-isopropyl ether (CAS No. 108-20-3)
Chemical name: Isopropyl ether; isopropoxy propane, 2-; oxybis [propane], 2,2 '-
Source/purity of test material: 98.5%
Conclusion : Under the conditions of this study, the test material was not mutagenic.
Reliability : (2) valid with restrictions
Restriction due to the lack of any information regarding the selection of dose levels used during the study. In addition no information is presented regarding cytotoxicity or the presence of test material precipitate in the cultures. Although study was not stated to be conducted under GLP, it was conducted at a reputable laboratory [Shell Research Limited, Sittingbourne Research Center].

10.11.2005 (4)

Type : Gene mutation in Saccharomyces cerevisiae
System of testing : Saccharomyces cerevisiae
Test concentration : Up to 8000 ug/ml in the pre-incubation mix
Cycotoxic concentr. :
Metabolic activation : with and without
Result : negative
Method : other: Similar to OECD Guideline 481
Year : 1984
GLP : no data
Test substance : other TS: Di-isopropyl ether (CAS No. 108-20-3)

Remark : Test type: Yeast mitotic gene conversion

Strains tested: JD1

Exposure method: [Brooks and Dean 1981]

Metabolic activation: With and without (S9 fraction mix of livers of Aroclor 1254 pretreated rats)

Vehicle: Tween 80/ethanol

Tester strain, activation status, Positive Controls and concentration level: Yeast cells were grown in log-phase, washed and resuspended in 2/5 strength YEPD broth at a concentration of 1 X 107 cells/ml. The suspension was divided into 1.9 ml amounts in 30 ml universal containers and 0.1 ml of test compound solution was added. For experiments with metabolic activation [+S9], 0.1 ml of DIPE was added to0 1.6 ml of yeast cell suspension, together with 0.3 ml of S9 mix. Initially a range of concentrations of DIPE was tested up to 5 mg/ml if solubility allowed. A second experiment was performed based on these results and taking into account cell viability. The cultures were incubated with shaking at 30 C for 18 hr. Aliquots were plated onto the appropriate culture media for selection of mitotic gene convertants and cells surviving the treatment. Mitotic gene

conversion may be scored by supplementing the minimal medium with histidine to score tryptophan prototrophs, and with tryptophan to score histidine prototrophs. Control plates were set up with solvent alone and with the positive control compounds 4-nitroquinoline oxide and cyclophosphamide.

Vehicle control: Yes

Dose rangefinding study: Cytotoxicity study

S9 Optimization study: No

Result : DIPE did not induce mitotic gene conversion I yeast. The test substance was not genotoxic in this assay with or without metabolic activation.

Test substance : Di-isopropyl ether (CAS No. 108-20-3)
Chemical name: Isopropyl ether; isopropoxy propane, 2-; oxybis [propane], 2,2 '-
Source/purity of test material: 98.5%

Conclusion : Under the conditions of this study, the test material was not genotoxic.

Reliability : (2) valid with restrictions
Restriction due to the lack of any information regarding the selection of dose levels used during the study. In addition no information is presented regarding cytotoxicity or the presence of test material precipitate in the cultures. Although study was not stated to be conducted under GLP, it was conducted at a reputable laboratory [Shell Research Limited, Sittingbourne Research Center].

10.11.2005 (4)

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species : rat
Sex : female
Strain : Sprague-Dawley
Route of admin. : inhalation
Exposure period : 6 hr/day
Frequency of treatm. : Gestation Days 6-15
Duration of test : 20 days
Doses : 0, 430, 3095, or 6745 ppm
Control group : other: yes (untreated & sham-exposed)
other: NOEL Maternal : = 430 ppm
other: NOEL Pup : = 430 - ppm
Result : Maternal NOEL: 430 ppm; Pup NOEL: 430 ppm
Method : EPA OTS 798.4350
Year : 1996
GLP : no data
Test substance : other TS: Diisopropyl Ether (CAS No. 108-20-3)

Method : Statistical method:
Statistical analyses of numerical data included ANOVA and Tukey's studentized range test for data on serum chemistry. Duncan's multiple

range test was used for hematology and body weights to assess statistically significant differences between control and exposed groups. Data on the maternal biophase, cesarean sections, and fetuses were evaluated by ANOVA followed by group comparisons using Fisher's exact or Dunnett's test.

Remark : Nulliparous females were housed with males in a 1:1 ratio and observed daily for evidence of breeding activity. Females positive for sperm plug and for sperm in the vaginal lavage fluid were considered to be at day 0 of gestation and were individually housed. The females were then randomly distributed to 5 groups of 22 animals each: untreated controls, sham-exposed controls, and 3 groups exposed to vapors of DIDP at 430, 3095, or 6745 ppm for 6 hr/day on gestation days (GD) 6-15.

Vapors were generated by metering DIPE on to a warmed fiberglass wick and carried to the three 1m3 exposure chambers by a stream of measured and filtered room air. Temperature and humidity in the chambers were measured every 30 minutes and air flow through each chamber was metered to provide at least 12 air changes/hour. Chamber air samples were collected with a gas-tight syringe and analyzed with a gas chromatograph with a flame ionization detector and a fused silica column. Samples were periodically obtained for analysis by gas chromatography/ mass spectroscopy.

Sham-exposed and test animals were housed in their exposure chambers throughout the exposure period; untreated controls in a separate room. Food and water were not available during the 6 -hour exposure periods but were available ad libitum at all other times. All animals were observed daily. Body weights were recorded on days 0, 6, 13, 16, and 20. Food consumption was measured on GD 6, 13, 16, and 20. Females were sacrificed on GD 20 by diethyl ether overexposure followed by exsanguination. Serum samples from the descending aorta were analyzed for glucose, urea nitrogen, total protein, albumin, globulin, A/G ratio, sorbitol dehydrogenase, lactate dehydrogenase, aspartate aminotransferase, alanine aminotransferase, alkaline phosphatase, total bilirubin, creatinine, cholesterol, triglycerides, uric acid, Cl, Ca, Na, K, and P. All organs were examined grossly. The number of corpora lutea per ovary and the gravid uterine weights were recorded. Uterine contents were examined and the numbers of implantation sites, early and late resorptions, and live and dead fetuses were recorded. The gender of each fetus was recorded. Fetuses were weighed and examined for gross anomalies. Fetuses of each litter were equally distributed between two groups; half were fixed in Bouin's solution and examined for visceral anomalies and the remaining fetuses were fixed in 95% ethanol and examined for skeletal anomalies after differential staining for cartilage and bone.

Dams exposed to 6745 ppm had a slight reduction in body weight gain and a significant decrease in food consumption. A concentration-related increase in the incidence of rudimentary 14th ribs was observed (statistically significant at 3095 and 6745 ppm) but the relevance of the finding was uncertain. There was no apparent toxicity, either maternal or fetal, at the lowest exposure concentration, 430 ppm.

Type: Developmental Toxicity
Species/strain: Sprague-Dawley; VAF/Plus Crl:CD(SD)BR
No./dose: 22/group
Vehicle: None
Method: USEPA 1984; 40CFR Part 798:4350

Result : Maternal NOEL: 430 ppm
Pup NOEL: 430 ppm

Test substance : Diisopropyl Ether (CAS No. 108-20-3); purity ~92%.

Conclusion : DIPE is not a teratogen.

Reliability : (2) valid with restrictions

GLP unknown. Study well documented, meets generally accepted scientific principles, acceptable for assessment.

01.11.2005 (8)

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

Type : other: Sensory Irritation in Humans

Method : Non-guideline.
Remark : Species/strain: Humans
Sex: Male and female
Number/sex/group: Average of 12
Route of administration: Inhalation
Vehicle: None
Control: No
Year: Prior to 1946
GLP: No
Result : 300 ppm: 35% of the subjects objected to this solvent because of the unpleasant odor rather than irritation.
500 ppm: there was a sensory response that was acceptable to the majority of subjects.
Test condition : Subjects were exposed for 15 minutes and olfactory fatigue and irritation of mucous membranes were reported. "Motion pictures were shown to occupy the subject's attention and divert their thoughts from the atmospheric contamination to which they were exposed."
Test substance : Diisopropyl ether (CAS No. 108-20-3)
Chemical Name: Isopropyl ether; isopropoxy propane, 2-; oxybis [propane], 2,2 '-
Test material is stated to be technical grade product.
Conclusion : DIPE does not appear to be a sensory irritant at concentrations up to 500 ppm, but it does have an unpleasant odor at this concentration.
Reliability : (2) valid with restrictions
Not GLP but conducted at a reputable laboratory [Harvard School of Public Health, Boston].

01.11.2005 (37)

Type : other: Sensory irritation in humans

Method : Non-Guideline.
Remark : Species/strain: Young adult humans [University of California staff and medical students]
Sex: Not specified
Number/sex/group: Not specified
Route of administration: Inhalation
Vehicle: None
Control: No
Year: 1955
GLP: No
Result : Numbers of subjects with degree of effect

		Concentration 400 ppm 800 ppm Number subjects: 7 7 Eye irritation: 7 absent 3 absent, 3 slight, 1 mod. Nose irritation: 5 absent, 2 slight 2 absent, 5 slight Pulmonary discomfort: 7 absent 4 absent, 3 slight Olfactory cognition : 1 slight, 6 mod. 4 mod., 3 severe CNS effects : 7 absent 7 absent
Test condition	:	Exposures were conducted in a whole-body chamber approximately 7700 l equipped with a fan. Exposures were made in a static atmosphere generated by vaporizing a predetermined quantity of test solvent from a hot surface. Five minutes were allowed for evaporation and equilibration, and subjects were exposed for 5 minutes, during which time they noted the degree of subjective responses at one-minute intervals.
Test substance	:	Diisopropyl ether (CAS No. 108-20-3) Chemical Name: Isopropyl ether; isopropoxy propane, 2-; oxybis [propane], 2,2 '- Test material is stated to be commercial grade with purity of 98% or better, provided by Shell Chemical Corporation.
Conclusion	:	400 ppm: 5 mins of inhalation exposure caused no eye irritation, none to slight nose irritation, no pulmonary discomfort, olfactory recognition but no central nervous system effects. 800 ppm: 5 mins of inhalation exposed caused slight eye and nose irritation, none to slight pulmonary discomfort, definite olfactory recognition but no central nervous system effects.
Reliability	:	(2) valid with restrictions Not GLP but conducted at a reputable laboratory [University of California School of Medicine].

01.11.2005 (22)

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

(1) Bridie A, Wolff C and Winter M (1979). The acute toxicity of some petrochemicals to goldfish. Water Res. 13:623-626.

(2) Bridié A, Wolff C and Winter M (1979). BOD and COD of some petrochemicals. Wat. Res. 13, 627-630.

(3) Broderius S, and Kahl M (1985). Acute toxicity of organic chemical mixtures to the fathead minnow. Aquat. Toxicol. 6:307-322.

(4) Brooks T.M., Meyer A.L. and Hutson D.H. (1988). The genetic toxicology of some hydrocarbon and oxygenated solvents. Mutagenesis, 3(3):227-232.

(5) Brooks TM, Meyer AL and Hutson DH (1988). The genetic toxicology of some hydrocarbon and oxygenated solvents. Mutagenesis 3(3):227-232.

(6) Cano M, Wilcox M and van Compernolle R (1999). A direct comparison of U.S. Environmental Protection Agency's Method 304B and batch tests for determining activated-sludge biodegradation rate constants for volatile organic compounds. Wat. Environ. Res. 71, 1345-1353.

(7) Church C and Tratnyek P (2000). Process level investigations of the in situ degradation of MTBE. Presented at the MTBE Biodegradation Workshop, February 1-3, 2000. Cincinnati, OH, USA.

(8) Dalbey W and Fueston M (1996). Subchronic and Developmental Toxicity Studies of Vaporized Diisopropyl Ether in Rats. Journal of Toxicology and Environmental Health 49:29-43.

(9) Daubert T and Danner R (1989). Physical and thermodynamic properties of pure chemicals: Data compilation. Design Institute for Physical Property Data, American Institute of Chemical Engineers. Hemisphere Publishing Corp., New York, NY, USA.

(10) Dawson G, Jennings A, Drozdowski D and Rider E (1975/77). The acute toxicity of 47 industrial chemicals to fresh and saltwater fishes. J. Haz. Mat. 1:303-318.

(11) Eadsforth C (1983). Isopropyl ether: determination of the n-octanol/water partition coefficient using a reverse-phase HPLC method. Report # SBGR.83.131. Shell Research Limited, Sittingbourne Research Centre, Sittingbourne, Kent, England.

(12) Eastern Research Group Inc. (2001). Summary of Workshop on Biodegradation of MTBE, February 1-3, 2000. Report No. EPA/625/R-01/001A, February, 2001.

(13) ECOSAR v0.99h in EPI Suite (2000). Estimation Program Interface Suite, v3.12. Syracuse Research Corporation, Syracuse, NY, USA.

(14) EPI SuiteTM (2000). Estimation Program Interface Suite, v3.12. Syracuse Research Corporation, Syracuse, NY, USA.

(15) EPIWIN (2000). Estimation Program Interface for Windows, version 3.12. Syracuse Research Corporation, Syracuse, NY, USA.

(16) Geiger D, Poirier S, Brooke L and Call D (eds.) (1986). Acute Toxicities of Organic Chemicals to Fathead Minnows (Pimephales promelas), Vol. 3. Center for Lake Superior Environmental Studies, Univ. of Wisconsin- Superior, Superior, WI, USA.

(17) Gerhartz W, Yamamoto Y, Kaudy L, Rounsaville J and Schulz G (eds.) (1987). Ullmann's Encyclopedia of Industrial Chemistry. Vol. A 10. 5th Edition. VCH Publishers, New York, NY, USA.

(18) Gould E (1959). Mechanism and Structure in Organic Chemistry. Holt, Reinhart and Winston, New York, NY, USA.

(19) Hansch C, Leo A and Hoekman D (1995). Exploring QSAR - Hydrophobic, Electronic and Steric Constants. p. 6. ACS Professional Reference Book, American Chemical Society, Washington, DC, USA.

(20) Harris J (1982). Rate of Hydrolysis. In: Handbook of Chemical Property Estimation Methods. Chapter 7. Edited by WJ Lyman, WF Reehl and DH Rosenblatt. McGraw-Hill Book Company, New York, NY, USA.

(21) Hernandez-Perez G, Fayolle F and Vandecasteele J-P (2001). Biodegradation of ethyl t-butyl ether (ETBE), methyl t-butyl ether (MTBE) and t-amyl methyl ether (TAME) by Gordonia terrae. Appl. Microbiol. Biotechnol. 55, 117-121.

(22) Hine CH, Anderson HH and Kodama JK (1955). Sensory thresholds of certain Shell organic solvents, Progress Report 1, Report to Shell Development Company, November 15, 1955. UC Report No. 247.

(23) Kimura ET, Ebert DM and Doge PW (1971). Acute toxicity and limits of solvent residues for sixteen organic solvents. Toxicol. Appl. Pharmacol. 19:699-704.

(24) Kropp K, Mormile M and Suflita J (2000). Anaerobic biodegradation of MTBE and alternative gasoline oxygenates. Presented at the MTBE Biodegradation Workshop, February 1-3, 2000. Cincinnati, OH, USA.

(25) Lide D, et al. (eds.) (1997-1998). CRC Handbook of Chemistry and Physics. 78th Edition. CRC Press, New York, NY, USA.

(26) Machle W, Scott EW and Treon J (1939). The physiological response to isopropyl ether and to a mixture of isopropyl ether and gasoline. J. Ind. Hyg. Toxicol. 21:72-96.

(27) Mackay D (1991). Multimedia Environmental Models; The Fugacity Approach. Lewis Publishers, CRC Press, pp 67-183.

(28) Mackay D (1998). Level I Fugacity-Based Environmental Equilibrium Partitioning Model, Version 2.1 (16-bit). Environmental Modelling Centre, Trent University, Ontario, Canada.

(29) Mackay D (2001). Multimedia Environmental Models: The Fugacity Approach - Second Edition. Lewis Publishers, Boca Raton, pp.1-261.

(30) Mackay D, et al (1996a). Assessing the fate of new and existing chemicals: a five-stage process. Environ. Toxicol. Chem. 15(9):1618-1626.

(31) Mackay D, et al (1996b). Evaluating the environmental fate of a variety of types of chemicals using the EQC model. Environ. Toxicol. Chem. 15(9):1627-1637.

(32) Mormile M, Liu S and Suflita J (1994). Anaerobic biodegradation of gasoline oxygenates: Extrapolation of information to multiple sites and redox conditions. Environ. Sci. Technol. 28, 1727-1732.

(33) Pruden A, Suidan M, Venosa A and Wilson G (2001). Biodegradaton of methyl tert-butyl ether under various substrate conditions. Environ. Sci. Technol. 35, 4235-4241.

(34) Rajagopalan S, van Compernolle R, Meyer M, Cano M, and Sun P (1998). Comparison of methods for determining biodegradation kinetics of volatile organic compounds. Water Environ. Res. 70, 291-298.

(35) Rodriguez SC and Dalbey W (1997). Subchronic neurotoxicity of vaporized Diisopropyl Ether in rats. International Journal of Toxicology 16:599-610.

(36) Scow K, Smith A, Leung J, Mackay D and Lory E (2000). Bioaugmentation of MTBE-contaminated groundwater with bacterial strain PM1. Presented at the MTBE Biodegradation Workshop, February 1-3, 2000. Cincinnati, OH, USA.

(37) Silverman LH, Schulte F and First MW (1946). Further studies on sensory response to certain industrial solvent vapors. J. Ind. Hyg. Toxicol. 28(6):262-266.

(38) Stephenson R (1983). Isopropyl Ether: Acute Toxicity to Daphnia magna and Selenastrum capricornutum. Group Research Limited, Report No. SBGR.83.215. Shell Research Ltd. Sittingbourne Research Centre, Sittingbourne, UK.

(39) Stephenson R (1983). Isopropyl ether: Acute toxicity to Daphnia magna and Selenastrum capricornutum. Report # SBGR.83.215, Shell Research Ltd. Sittingbourne Research Centre, Sittingbourne, Kent, England.

(40) Stone C and Watkinson R (1983). Isopropyl ether: An assessment of ready biodegradability. Report # SBGR.83.428. Shell Biosciences Laboratory, Sittingbourne Research Centre, Sittingbourne, Kent, England.

(41) Suflita J and Mormile M (1993). Anaerobic biodegradation of known and potential gasoline oxygenates in the terrestrial subsurface. Environ. Sci. Technol. 27, 976-978.

(42) U.S. EPA. (1994). Method 304B - Determination of biodegradation rates of organic compounds (scrubber option). Appendix A to Part 63 - Test Methods. Fed. Regist. 59,78, 19594.

(43) Veith G, Call D and Brooke L (1983). Structure-Toxicity Relationships for the Fathead Minnow, Pimephales promelas: Narcotic Industrial Chemicals. Can. J. Fish. Aquat. Sci. 40, 743-748.

(44) Wass U and Belin L (1990). An in vitro method for predicting sensitizing properties of inhaled chemicals. Scand. J. Work Environ. Health. 116:208-214.

(45) Zenker M, Borden R, and Barlaz M (1999). Investigation of the intrinsic biodegradation of alkyl and cyclic ethers. Vol. 1, pp 165-170, 5th Int. In Situ On-Site Biorem. Symp.

(46) Zepp R and Cline D (1977). Rates of direct photolysis in the aqueous environment. Environ. Sci. Technol. 11:359-366.

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

IUCLID

Data Set

Existing Chemical	:	ID: 78-92-2
CAS No.	:	78-92-2
EINECS Name	:	butan-2-ol
EC No.	:	201-158-5
TSCA Name	:	2-Butanol
Molecular Formula	:	C4H10O

Producer related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	09.01.2002

Substance related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	09.01.2002
Status	:	
Memo	:	
Printing date	:	01.06.2006
Revision date	:	
Date of last update	:	01.06.2006
Number of pages	:	76
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

Type	:	
Name	:	Atochem
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Telex	:	
Cedex	:	
Email	:	
Homepage	:	

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA) 11.02.2000

Type	:	
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Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA) 11.02.2000

Type	:	
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Town	:	PO15 7AP Fareham, Hampshire
Country	:	United Kingdom
Phone	:	(44)489.88.4480
Telefax	:	(44)489.88.4455
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA) 11.02.2000

Type	:	
Name	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Contact person	:	
Date	:	
Street	:	Ueberseering 40
Town	:	22297 Hamburg

Country	:	Germany
Phone	:	040-6375-0
Telefax	:	040-6375-3496
Telex	:	21151320
Cedex	:	
Email	:	
Homepage	:	

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

Type	:	
Name	:	SHELL FRANCE
Contact person	:	
Date	:	
Street	:	89 bld Franklin Roosevelt
Town	:	92564 Rueil Malmaison
Country	:	France
Phone	:	33 1 47.14.71.00
Telefax	:	33 1 47.14.82.99
Telex	:	SHELL 615013F
Cedex	:	
Email	:	
Homepage	:	

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

Type	:	
Name	:	Shell Nederland Chemie B.V.
Contact person	:	
Date	:	
Street	:	P.O. Box 3030
Town	:	3190 GH Hoogvliet-Rotterdam
Country	:	Netherlands
Phone	:	+31-10-2317005
Telefax	:	+31-10-2317125
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

Type	:	
Name	:	Union Carbide Benelux
Contact person	:	
Date	:	
Street	:	Norderlaan 147
Town	:	2030 Antwerpen
Country	:	Belgium
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type :
Substance type : organic
Physical status : liquid
Purity :
Colour :
Odour :

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

2-Butanol

Source : Shell Nederland Chemie B.V. Hoogvliet-Rotterdam
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
19.05.1994

2-butanol

Source : Union Carbide Benelux Antwerpen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
26.05.1994

2-Hydroxybutane

Source : Shell Nederland Chemie B.V. Hoogvliet-Rotterdam
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
19.05.1994

butan-2-ol

Source : EXXON CHEMICAL, Limited Fareham, Hampshire
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
16.02.1994

Ethyl methyl carbinol

Source : Shell Nederland Chemie B.V. Hoogvliet-Rotterdam
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
19.05.1994

SBA

Source : EXXON CHEMICAL, Limited Fareham, Hampshire
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
16.02.1994

SBA; sec-Butanol; Butan-2-ol; secondary butyl alcohol

Source : Atochem Paris la Defense
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
27.04.1994

SBA; secondary butyl alcohol; ethyl methyl carbinol; 2-hydroxybutane

Source : SHELL FRANCE Rueil Malmaison
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
20.05.1994

sec-butanol

Source : Union Carbide Benelux Antwerpen
EXXON CHEMICAL, Limited Fareham, Hampshire
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
26.05.1994

sec.-butyl alcohol, iso-butanol

Source : Deutsche Shell Chemie GmbH Eschborn
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
30.05.1994

secondary butyl alcohol

Source : EXXON CHEMICAL, Limited Fareham, Hampshire
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
16.02.1994

secundary butyl alcohol

Source : Union Carbide Benelux Antwerpen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
26.05.1994

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

Quantity : 100000 - 500000 tonnes in

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

1.6.1 LABELLING

Labelling : as in Directive 67/548/EEC
Specific limits : no data
Symbols : Xi, , ,
Nota : C, C,
R-Phrases : (10) Flammable
(36/37) Irritating to eyes and respiratory system
(67) Vapours may cause drowsiness and dizziness
S-Phrases : (2) Keep out of reach of children
(7/9) Keep container tightly closed and in a well-ventilated place
(13) Keep away from food, drink and animal feeding stuffs
(24/25) Avoid contact with skin and eyes
(26) In case of contact with eyes, rinse immediately with plenty of water and seek medical advice
(46) If swallowed, seek medical advice immediately and show this container or label

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

1.6.2 CLASSIFICATION

Classified : as in Directive 67/548/EEC
Class of danger : irritating
R-Phrases : (36/37) Irritating to eyes and respiratory system
Specific limits :

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

Classified : as in Directive 67/548/EEC
Class of danger :
R-Phrases : (10) Flammable
Specific limits :

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

Classified : as in Directive 67/548/EEC
Class of danger :
R-Phrases : (67) Vapours may cause drowsiness and dizziness
Specific limits :

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

1.6.3 PACKAGING

1.7 USE PATTERN

Type of use : type
Category : Non dispersive use

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

Type of use : type
Category : Use in closed system

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

Type of use : type
Category : Use resulting in inclusion into or onto matrix

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

Type of use : type
Category : Wide dispersive use

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

Type of use : industrial
Category : Basic industry: basic chemicals

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

Type of use : industrial
Category : Chemical industry: used in synthesis

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

Type of use : industrial
Category : Fuel industry

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

Type of use : industrial
Category : Paints, lacquers and varnishes industry

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

Type of use : use
Category : Intermediates

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

Type of use : use

Category : Solvents

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

Type of use : use
Category : other: fuel additive in lead-free gasoline

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

Type of use : use
Category : other

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

Type of limit : MAC (NL)
Limit value : 450 mg/m3

Source : Shell Nederland Chemie B.V. Hoogvliet-Rotterdam
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
03.06.1994 (29)

Type of limit : MAC (NL)
Limit value : 450 mg/m3

Source : EXXON CHEMICAL, Limited Fareham, Hampshire
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
16.02.1994

Type of limit : MAC (NL)
Limit value : 450 mg/m3

Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
13.05.1994

Type of limit : MAK (DE)
Limit value : 300 mg/m3
Short term exposure limit value
Limit value : 600 mg/m3
Time schedule : 30 minute(s)
Frequency : 4 times

Source : Atochem Paris la Defense

EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
27.04.1994 (53)

Type of limit : MAK (DE)
Limit value : 300 mg/m3

Source : EXXON CHEMICAL, Limited Fareham, Hampshire
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
16.02.1994

Type of limit : MAK (DE)
Limit value : 100 ml/m3

Remark : Substance is easily resorbed.
Source : Deutsche Shell Chemie GmbH Eschborn
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
30.05.1994

Type of limit : OES (UK)
Limit value : 300 mg/m3
Short term exposure limit value
Limit value : 450 mg/m3
Time schedule :
Frequency : times

Source : EXXON CHEMICAL, Limited Fareham, Hampshire
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
16.02.1994

Type of limit : TLV (US)
Limit value : 303 mg/m3

Source : Shell Nederland Chemie B.V. Hoogvliet-Rotterdam
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
03.06.1994 (3)

Type of limit : TLV (US)
Limit value : 303 mg/m3
Short term exposure limit value
Limit value : 455 mg/m3
Time schedule :
Frequency : times

Source : Union Carbide Benelux Antwerpen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
26.05.1994 (1)

Type of limit : TLV (US)
Limit value : 303 mg/m3
Short term exposure limit value
Limit value : 455 mg/m3
Time schedule : 15 minute(s)
Frequency : 4 times

Source : Atochem Paris la Defense
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
27.04.1994 (53)

Type of limit : TLV (US)
Limit value : 303 mg/m3

Remark : Use local exhaust ventilation.
Hand protection : PVC, nitrile or neoprene gloves.
Eye protection : safety monogoggles.
Body protection : standard issue work clothes.
chemicals resistant safety shoes or boots.
Source : SHELL FRANCE Rueil Malmaison
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
26.05.1994 (88)

Type of limit : TLV (US)
Limit value : 303 mg/m3
Short term exposure limit value
Limit value : 455 mg/m3
Time schedule : 8 hour(s)
Frequency : times

Source : EXXON CHEMICAL, Limited Fareham, Hampshire
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
16.02.1994

Type of limit : other: VME
Limit value : 300

Country : France
Source : Atochem Paris la Defense
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
27.04.1994 (52)

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

Remark : As the quantities of this substance placed on the EU market by Union Carbide Benelux N.V. are normally sourced from the manufacturing facilities of its U.S. parent company, no exposure can arise within the EU from the manufacture of these substances. The comments below on exposure are restricted to uses for which Union Carbide believes its customers use this substance.

Major use(s): Fuel additive in lead-free gasoline.

Sources of human exposure: Very minor sporadic exposure to the public via inhalation during filling of vehicles. Quantitative estimates are not available.

Sources of environmental exposure: Negligible sporadic exposure to the atmosphere during filling of vehicles. Quantitative estimates are not available. Substance is essentially oxidised to carbon dioxide and water during use.

Source : Union Carbide Benelux Antwerpen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

24.05.1994

Remark : Continuous process. Non-direct hydratation by absorption of butenes in sulfuric acid.
One production site.
Distribution pattern : from production
% to air 0.02
% to water 0.02
to soil 0.0
to sediment 0.0

Source : Atochem Paris la Defense
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

03.06.1994

Remark : Inhalation or skin contact when loading, unloading, using the product.
In case of accidental release, product may contaminate the environment.

Source : SHELL FRANCE Rueil Malmaison
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

23.02.1994

1.11 ADDITIONAL REMARKS

Remark : DISPOSAL

Recover or recycle if possible. Otherwise incineration.

TRANSPORT INFORMATION

UN Number: 1120
Class: 3
Packing Group: III
Proper Shipping Name: Secondary butyl alcohol

Sea (IMO)
Class: 3.3
Packing Group: III
Symbol: Flammable liquid
Marine Pollutant (Y/N): No

Rail/Road (RID/ADR)
Class: 3
Item: 31(c)
Symbol: Flammable liquid
Kemler Plate: 30/1120

Air (IATA/ICAO)
Class: 3
Packing Group: III
Symbol: Flammable liquid

Source : Shell Nederland Chemie B.V. Hoogvliet-Rotterdam
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

10.06.1994

Remark : Disposal: Incinerate in a furnace where permitted under national and local regulations.

Transport: Butan-2-ol is classified as a class 3 product according the ADR/RID/IMDG/ICAO regulations.
Butan-2-ol is shipped in road/rail tankcars, tankcontainers/ISOtanks and smaller packages (e.g. drums).
¿

Source : Union Carbide Benelux Antwerpen
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

26.05.1994

Remark : Recover or recycle if possible. Otherwise : incineration.
Avoid electrostatic discharge generation.
Earth all equipment.
Avoid splash filling.
Use a vapour recovery system.
Keep in a well ventilated place.
Avoid naked flames. Remove ignition sources.
Do not smoke. Avoid sparks.
Transport

UN number : 1120
Class : 3
Packing Group : III
Proper Shipping Name : Secondary butyl alcohol

Sea (IMO)
Class : 3.3
Marine Pollutant : No
Symbol : Flammable liquid

Rail/Road (ADR/RID)
Class : 3
Item : 31 c)
Symbol : Flammable liquid
Kemler Plate : 30/1120

Air (IATA/IACO)

Class : 3
Symbol : Flammable liquid

Source : SHELL FRANCE Rueil Malmaison
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

26.05.1994

Remark : Disposal options:
Recover or recycle if possible. Otherwise: incineration.

Transport classification:

UN number: 1120
ADR/RID:
class/item: 3/31 c
packing group: 3
Kemler number: 30
label: 3
Proper shipping name: sec.-butyl alcohol

ICAO:
class: 3
packing group: III
label: flammable liquid
Proper shipping name: butanols

IMO/IMDG:
class: 3.3
packing group: III
Marine pollutant: no
label: flammable liquid
IMDG page: 3313
EMS number: 3-06
MFAG plate: 305

Source : Deutsche Shell Chemie GmbH Eschborn
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

30.05.1994

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value	:	= -114 °C
Sublimation	:	
Method	:	other: no data
Year	:	
GLP	:	no data
Test substance	:	
Remark	:	Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.
Source	:	ExxonMobil Biomedical Sciences, Inc., New Jersey, USA

17.01.2002 (50)

Value	:	ca. -89 - -108 °C
Sublimation	:	
Method	:	other: no data
Year	:	
GLP	:	no data
Test substance	:	
Remark	:	Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.
Source	:	EXXON CHEMICAL, Limited Fareham, Hampshire EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

17.01.2002 (57)

2.2 BOILING POINT

Value	:	= 99.5 °C at
Decomposition	:	
Method	:	other: no data
Year	:	
GLP	:	no data
Test substance	:	
Remark	:	Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.
Source	:	ExxonMobil Biomedical Sciences, Inc., New Jersey, USA

17.01.2002 (38)

Value	:	ca. 99 - 102 °C at 1013 hPa
Decomposition	:	
Method	:	other: ASTM D1078/86
Year	:	1986
GLP	:	no data
Test substance	:	
Remark	:	Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.
Source	:	ExxonMobil Biomedical Sciences, Inc., New Jersey, USA EXXON CHEMICAL, Limited Fareham, Hampshire EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

17.01.2002

2.3 DENSITY

Type : density
Value : = 806 kg/m3 at 20 °C
Method : other: no data
Year :
GLP : no data
Test substance :

Remark : Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.
Source : ExxonBiomedical Sciences, Inc., New Jersey, USA
17.01.2002 (23)

Type : density
Value : ca. 807 kg/m3 at 15 °C
Method : other: ASTM D4052/86
Year : 1986
GLP : no data
Test substance :

Source : EXXON CHEMICAL, Limited Fareham, Hampshire
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
17.01.2002 (39)

Type : density
Value : = 3.29 kg/m3 at 20 °C
Method : other: no data
Year :
GLP : no data
Test substance :

Remark : Vapour density
Source : EXXON CHEMICAL, Limited Fareham, Hampshire
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
17.01.2002 (76)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : = 15.98 hPa at 20 °C
Decomposition :
Method : other (measured)
Year :
GLP : no data
Test substance :

Remark : Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.
Source : EXXON CHEMICAL, Limited Fareham, Hampshire
ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
17.01.2002 (57)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	
Log pow	:	= .61 at 20 °C
pH value	:	
Method	:	other (measured)
Year	:	
GLP	:	no data
Test substance	:	
Remark	:	Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.
Source	:	ExxonMobil Biomedical Sciences, Inc., New Jersey, USA

17.01.2002 (47)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	
Value	:	= 125 g/l at 20 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: no data
Year	:	
GLP	:	no data
Test substance	:	
Remark	:	Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.
Source	:	EXXON CHEMICAL, Limited Fareham, Hampshire ExxonMobil Biomedical Sciences, Inc., New Jersey, USA EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

17.01.2002 (46)

Solubility in	:	
Value	:	= 181 g/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: no data
Year	:	
GLP	:	no data
Test substance	:	
Remark	:	Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.
Source	:	ExxonMobil Biomedical Sciences, Inc., New Jersey, USA

17.01.2002 (51)

Solubility in	:	
Value	:	ca. 201 g/l at 20 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: no data
Year	:	
GLP	:	no data
Test substance	:	
Remark	:	Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.
Source	:	EXXON CHEMICAL, Limited Fareham, Hampshire ExxonMobil Biomedical Sciences, Inc., New Jersey, USA EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

17.01.2002 (57)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value	:	= 24 °C
Type	:	closed cup
Method	:	other: NFT 60 103
Year	:	
GLP	:	no data
Test substance	:	
Remark	:	Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.
Source	:	EXXON CHEMICAL, Limited Fareham, Hampshire ExxonMobil Biomedical Sciences, Inc., New Jersey, USA EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

17.01.2002 (74)

Value	:	ca. 25 °C
Type	:	closed cup
Method	:	Directive 84/449/EEC, A.9 "Flash point"
Year	:	1987
GLP	:	no data
Test substance	:	
Source	:	EXXON CHEMICAL, Limited Fareham, Hampshire EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

01.06.1994

2.8 AUTO FLAMMABILITY

Value	:	> 350 °C at 1013 hPa
Method	:	other: E695/85
Year	:	1985
GLP	:	no data

Test substance :

Remark : Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.
Source : EXXON CHEMICAL, Limited Fareham, Hampshire
ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
17.01.2002 (39)

Value : = 406 °C at 1013 hPa
Method : other: no data
Year :
GLP : no data
Test substance :

Source : EXXON CHEMICAL, Limited Fareham, Hampshire
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
02.06.1994 (75)

2.9 FLAMMABILITY

Result : flammable
Method : other: no data
Year :
GLP : no data
Test substance :

Remark : Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.
Source : EXXON CHEMICAL, Limited Fareham, Hampshire
ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
17.01.2002 (74)

2.10 EXPLOSIVE PROPERTIES

Method : other: no data
Year :
GLP : no data
Test substance :

Remark : Explosive limits of vapours in air: 1.7 to 9.8% vol.
Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.
Source : EXXON CHEMICAL, Limited Fareham, Hampshire
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
17.01.2002 (74)

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000 molecule/cm³
Rate constant	:	= .0000000000099751 cm³/(molecule*sec)
Degradation	:	= 50 % after 12.9 hour(s)
Deg. product	:	
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	
Remark	:	50% degradation after 1.07 days based on a 12-hr. day. The SMILES (Simplified Molecular Input Line Entry System) structure used with the model was: OC(CC)C. Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.
Source	:	ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
Reliability	:	(2) valid with restrictions Rated a 2 for reliability because it is a calculated value.

17.01.2002 (37)

Type	:	air
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	
Rate constant	:	cm³/(molecule*sec)
Degradation	:	% after
Deg. product	:	
Method	:	other (measured)
Year	:	
GLP	:	no data
Test substance	:	
Remark	:	Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%. Rate constants were determined from data developed in three labs. Two equations were applied to the measured data and designated the TI (time-included) and TE (time-excluded) methods. Both equations are in the form of a straight line equation, y=mx+b. Least square linear regression analyses were applied to the data from each experiment.
Result	:	Hydroxyl rate constants as calculated from measured data using the time-included equation: 10.30 +/- 2.48 x 10-12 cm3/molecule-sec (r2 = 0.97); @ 24C 11.55 +/- 1.77 x 10-12 cm3/molecule-sec (r2 = 0.99); @ 24C 4.01 +/- 1.38 x 10-12 cm3/molecule-sec (r2 = 0.76); @ 34C Hydroxyl rate constants as calculated from measured data using the time-excluded equation:

9.40 +/- 0.87 x 10-12 cm3/molecule-sec (r2 = 0.99); @ 24C
7.37 +/- 1.65 x 10-12 cm3/molecule-sec (r2 = 0.99); @ 24C
2.71 +/- 0.20 x 10-12 cm3/molecule-sec (r2 = 0.97); @ 34C

Source : ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
EXXON CHEMICAL, Limited Fareham, Hampshire
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
17.01.2002 (30)

Type : air
Light source :
Light spectrum : nm
Relative intensity : based on intensity of sunlight
INDIRECT PHOTOLYSIS
Sensitizer : OH
Conc. of sensitizer : 1000000 molecule/cm³
Rate constant : = .0000000000096466 cm³/(molecule*sec)
Degradation : = 50 % after 20 hour(s)
Deg. product :
Method : OECD Guide-line draft "Photochemical Oxidative Degradation in the Atmosphere"
Year : 1990
GLP :
Test substance :

Remark : Calculated value using draft OECD method of Atkinson (1990).
Source : EXXON CHEMICAL, Limited Fareham, Hampshire
ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
17.01.2002 (81)

Type : air
Light source : other: sun lamp
Light spectrum : nm
Relative intensity : based on intensity of sunlight
Deg. product :
Method : other (measured)
Year :
GLP : no data
Test substance :

Remark : Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.
Under simulated atmospheric conditions and in the presence of 5 ppm NO, the half life of 2-butanol (10 ppm) is 4 hours.
Source : EXXON CHEMICAL, Limited Fareham, Hampshire
ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
17.01.2002 (26)

Remark : 2-Butanol does not contain chromophores that adsorb light at wavelengths >290 nm. Therefore, direct photolysis will not occur.
Source : EXXON CHEMICAL, Limited Fareham, Hampshire
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
18.01.2002 (20)

3.1.2 STABILITY IN WATER

Type : abiotic
t1/2 pH4 : at °C

t1/2 pH7	:	at °C
t1/2 pH9	:	at °C
Deg. product	:	
Method	:	
Year	:	
GLP	:	no data
Test substance	:	

Result	:	Hydrolysis will not contribute to the transformation of sBA in aquatic environments. Hydrolysis of an organic chemical is the transformation process in which a water molecule or hydroxide ion reacts to form a new carbon-oxygen bond, thereby changing the parent chemical. Chemicals that are susceptible to hydrolysis contain functional groups that can be displaced by a nucleophilic substitution reaction. Simple alcohols such as sBA are resistant to hydrolysis because they lack a functional group that is hydrolytically reactive.
Source	:	EXXON CHEMICAL, Limited Fareham, Hampshire ExxonMobil Biomedical Sciences, Inc., New Jersey, USA EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

17.01.2002 (49)

3.1.3 STABILITY IN SOIL

Remark	:	If released on land, 2-butanol has the potential to leach into soil. 2-Butanol also has the potential to volatilize from dry soil. The estimated log Koc for 2-butanol is 0.84. Therefore, 2-butanol should not absorb significantly to soil or sediment. The Koc value was calculated using the equation in Lyman (1982): log Koc = -0.55log S + 3.64 (S, water solubility, in mg/L); water solubility value used = 125,000 mg/L from Hahn et al. (1986) [Lyman, W.J. (1982). Adsorption Coefficient for Soils and Sediments. In: Handbook of Chemical Property Estimation Methods. Environmental Behavior of Organic Compounds. 4,1-33. Lyman W.J., Reehl, W.F., and Rosenblatt, D.H. (eds). McGraw-Hill, New York, NY, USA.] [Hahn, H-D., Dämbkes, G., and Rupprich, N. (1986). Butanols. In: Gerhartz W (ed), Ullmann's encyclopedia of industrial chemistry, 5th ed, vol A4, benzyl alcohol to calcium sulfate. VCH, Weinheim, 463-474.]
Source	:	EXXON CHEMICAL, Limited Fareham, Hampshire ExxonMobil Biomedical Sciences, Inc., New Jersey, USA EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

18.01.2002 (62) (87)

3.2.1 MONITORING DATA

Type of measurement	:	background concentration
Media	:	surface water
Concentration	:	
Method	:	

Remark	:	2-Butanol has been detected in the Niagara River (Lake Ontario basin), but not in the western basin of Lake Ontario.
Source	:	EXXON CHEMICAL, Limited Fareham, Hampshire EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

17.01.2002 (43)

Type of measurement : background concentration
Media : air
Concentration :
Method :

Remark : 2-Butanol was detected but not quantified in forest air in the southern Black Forest of Germany.
Source : EXXON CHEMICAL, Limited Fareham, Hampshire
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
17.01.2002 (56)

Type of measurement : background concentration
Media : air
Concentration :
Method :

Remark : Low molecular weight alcohols, including 2-butanol, were not detected in air or precipitation samples taken at Tucson, Arizona, and two rural sites 40 km away.
Source : EXXON CHEMICAL, Limited Fareham, Hampshire
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
17.01.2002 (84)

Type of measurement : concentration at contaminated site
Media : other: wastewater
Concentration :
Method :

Remark : In a comprehensive survey of wastewater from 4000 industrial and publically owned treatment works sponsored by the Effluent Guidelines Division of the U.S. EPA, 2-butanol was identified in discharges of the following industrial category (positive occurences, median concentration in ppb): leather tanning (1; 46.7), petroleum refining (1; 149.3), paint and ink (1; 324.7), organics and plastics (2; 35.4), pesticides manufacture (1; 36.2), pharmaceuticals (1; 4.6), foundries (1; 41.0), electronics (1; 19.9), mechanical products (3; 90.6), publically owned treatment works (3; 12.4). The highest effluent concentration was 920.1 ppb in the mechanical products industry.
Source : EXXON CHEMICAL, Limited Fareham, Hampshire
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
17.01.2002 (80)

Type of measurement : concentration at contaminated site
Media : other: landfill leachate
Concentration :
Method :

Remark : 2-Butanol was found in landfill leachate from 1 of 5 sites in Connecticut. The concentration in this leachate ranged from 6.2 to 14.9 ppm.
Source : EXXON CHEMICAL, Limited Fareham, Hampshire
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
17.01.2002 (78)

Type of measurement : background concentration
Media : drinking water
Concentration :
Method :

Remark : 2-Butanol was identified in drinking water from Ottumwa, IA.
Source : EXXON CHEMICAL, Limited Fareham, Hampshire
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

17.01.2002 (61)

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : volatility
Media : water - air
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other
Year :

Result : On the basis of Henry's Law constant, the volatilization half-life of 2-butanol is estimated to be 120.2 hours in a model river with the follwoing parameters: 1 m deep, 1 m/sec flow rate, and 3 m/sec wind speed.
Source : EXXON CHEMICAL, Limited Fareham, Hampshire
ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

17.01.2002 (86)

3.3.2 DISTRIBUTION

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level I
Year :

Remark : Physicochemical data used in the calculation:

Parameter	Value w/ Units
Molecular Weight	74.12
Temperature	20 C
Log Kow	0.61
Water Solubility	125,000 g/m3
Vapor Pressure	1600 Pa
Melting Point	-114 C

Result : Using the Mackay Level I calculation, the following distribution is predicted for 2-butanol:

%Distribution	Compartment
16.28	Air
83.68	Water
0.03	Soil
0.01	Sediment
0.00	Suspended Sediment
0.00	Biota

Source : EXXON CHEMICAL, Limited Fareham, Hampshire
ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability : (2) valid with restrictions
Rated 2 for reliability due to calculated value.

17.01.2002 (64)

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type	:	aerobic
Inoculum	:	other: Wastewater treatment plant
Contact time	:	5 day(s)
Degradation	:	= 83 (±) % after 5 day(s)
Result	:	
Deg. product	:	
Method	:	other: APHA (American Public Health Association) Standard Methods, No. 219
Year	:	
GLP	:	no data
Test substance	:	
Method	:	The APHA No. 219 test method, which measures dissolved oxygen, is similar to the OECD 301D, Closed Bottle biodegradation test procedure.
Remark	:	Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.
Result	:	The ThOD (theoretical oxygen demand) = 2.59 g/g. The measured BOD (biological oxygen demand) = 2.15 g/g. The only deviation to the test method was that 0.5 mg/L of allylthiourea was added to the test medium to prevent nitrification.
Source	:	ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
Test condition	:	10 ml of filtered wastewater was used as an inoculum with 500 ml of test medium. The source of the inoculum from within the wastewater treatment plant was not stated. The inoculum was not acclimated. There was no information on controls and replicate test samples. Test temperature was 20 +/- 1 deg C.
Reliability	:	(2) valid with restrictions Although it was cited that a standard method was followed, there is little information in the article confirming that the test was conducted according to the method description. This lack of information supports a reliability rating of 2.

18.01.2002 (6)

Type	:	
Inoculum	:	other: Wastewater treatment plant
Contact time	:	50 day(s)
Degradation	:	(±) % after
Result	:	
Deg. product	:	
Method	:	other: Winkler Method
Year	:	
GLP	:	no data
Test substance	:	
Method	:	The Winkler method, which measures dissolved oxygen, is equivalent to the OECD 301D, Closed Bottle biodegradation test procedure.
Remark	:	Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.
Result	:	Day % Biodegradation (ThOD)

Day	% Biodegradation (ThOD)
5	0.0
10	44.2
15	69.2

		20 72.3
		30 73.2
		40 75.4
		50 77.0
Source	:	ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
Test condition	:	An azide modification of the Winkler test method was used. The source of the inoculum from within the wastewater treatment plant was not stated. There was no information on controls and replicate test samples. Test material loading was 2.5 ppm. Test temperature was 20 deg C.
Reliability	:	(2) valid with restrictions There is little information in the article describing how the study was conducted. This lack of information supports a reliability rating of 2. The results were comparable to reported data (Bridie, A.L., C.J.M. Wolff, and M. Winter. 1979. BOD and COD of Some Petrochemicals. Water Research. 13:627-630), which supports the acceptability of this study.

18.01.2002 (59)

Type	:	aerobic
Inoculum	:	activated sludge
Contact time	:	
Degradation	:	= 98.5 (±) % after 5 day(s)
Result	:	
Deg. product	:	
Method	:	other: screening test
Year	:	
GLP	:	no data
Test substance	:	
Remark	:	Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.
Source	:	EXXON CHEMICAL, Limited Fareham, Hampshire ExxonMobil Biomedical Sciences, Inc., New Jersey, USA EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

17.01.2002 (71)

Type	:	aerobic
Inoculum	:	activated sludge
Contact time	:	
Degradation	:	= 81.7 (±) % after 5 day(s)
Result	:	
Deg. product	:	
Method	:	other: screening test
Year	:	
GLP	:	no data
Test substance	:	
Remark	:	Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.
Source	:	EXXON CHEMICAL, Limited Fareham, Hampshire ExxonMobil Biomedical Sciences, Inc., New Jersey, USA EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

17.01.2002 (90)

Type	:	aerobic
Inoculum	:	activated sludge
Contact time	:	
Degradation	:	= 33 (±) % after 5 day(s)
Result	:	
Deg. product	:	
Method	:	other: screening test
Year	:	

GLP	:	no data
Test substance	:	
Remark	:	Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.
Source	:	EXXON CHEMICAL, Limited Fareham, Hampshire ExxonMobil Biomedical Sciences, Inc., New Jersey, USA EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA) 17.01.2002 (28)
Type	:	aerobic
Inoculum	:	activated sludge
Contact time	:	
Degradation	:	= 9.3 (±) % after 1 day(s)
Result	:	
Deg. product	:	
Method	:	other: screening test
Year	:	
GLP	:	no data
Test substance	:	
Remark	:	Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.
Source	:	EXXON CHEMICAL, Limited Fareham, Hampshire ExxonMobil Biomedical Sciences, Inc., New Jersey, USA EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA) 17.01.2002 (42)
Type	:	aerobic
Inoculum	:	other: semi-automatic activated sludge system
Contact time	:	
Degradation	:	(±) % after
Result	:	other: 98% BOD reduction after 5 days
Deg. product	:	
Method	:	
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	98% BOD reduction after 5 days
Source	:	EXXON CHEMICAL, Limited Fareham, Hampshire EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA) 14.01.2002 (77)
Type	:	anaerobic
Inoculum	:	other: acetate enriched cultures
Deg. product	:	
Method	:	
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	In a long-term study using anaerobic upflow filters, 93% utilization rate was seen after a 52 day operation.
Source	:	EXXON CHEMICAL, Limited Fareham, Hampshire EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA) 14.01.2002 (21)
Type	:	anaerobic
Inoculum	:	other: acetate-acclimated methane cultures
Contact time	:	
Degradation	:	100 (±) % after 14 day(s)

Result	:	
Deg. product	:	
Method	:	
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	EXXON CHEMICAL, Limited Fareham, Hampshire EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

14.01.2002 (92)

3.6 BOD5, COD OR BOD5/COD RATIO

BOD5		
Method	:	other: not specified
Year	:	
Concentration	:	related to
BOD5	:	= 1.87 mg/l
GLP	:	no data
COD		
Method	:	other: not specified
Year	:	
COD	:	= 2.47 mg/g substance
GLP	:	no data
RATIO BOD5 / COD		
BOD5/COD	:	= .76
Remark	:	Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.
Source	:	EXXON CHEMICAL, Limited Fareham, Hampshire ExxonMobil Biomedical Sciences, Inc., New Jersey, USA EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

17.01.2002 (57)

3.7 BIOACCUMULATION

BCF	:	ca. 1.71
Elimination	:	
Method	:	other: calculated value
Year	:	
GLP	:	no data
Test substance	:	
Remark	:	A bioconcentration factor of 1.7 is calculated using a 2-butanol log octanol/water partition coefficient (Kow) of 0.61 as reported by Hansch et al., 1995 (Hansch, C., Leo, A., Hoekman, D. 1995. Exploring QSAR - Hydrophobic, Electronic, and Steric Constants. American Chemical Society, Washington, DC, USA.).
Source	:	EXXON CHEMICAL, Limited Fareham, Hampshire ExxonMobil Biomedical Sciences, Inc., New Jersey, USA EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

18.01.2002 (16)

3.8 ADDITIONAL REMARKS

Memo	:	The volatilization half-life in a model river is estimated to be 3.5 days at 25 degrees C.

Source : EXXON CHEMICAL, Limited Fareham, Hampshire
ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

17.01.2002 (86)

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	flow through
Species	:	Pimephales promelas (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	= 3670 measured/nominal
Limit test	:	
Analytical monitoring	:	yes
Method	:	other: no data
Year	:	1985
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4

Method : The test method used in this study is similar to the OECD 203 test guideline.
Trimmed Spearman-Karber Method (Hamilton, M.A., R.C. Russo, and R.V. Thurston. 1977. Trimmed Spearman-Karber Method for Estimating Median Lethal Concentrations in Toxicity Bioassays. Environ. Sci. Technol. 11:714-719. Correction, 12:417, 1978.)

Remark : Purity: 99%

Result : 96-hour LC50 = 3,670 mg/L (95% CI 3,380 to 3,990) based upon average, corrected measured values
Analytical method used was Gas-Liquid Chromatography

Measured Conc. (mg/L)	Fish Total Mortality (@96 hrs)*
Control	0
1,018	0
1,839	0
2,630	0
4,258	16
6,667	20

* 20 fish added at test initiation

Source : ExxonMobil Biomedical Sciences, Inc., New Jersey, USA

Test condition : Treatment solutions were prepared by diluting a 3.7 g/L stock solution. Nominal sBA treatment levels were 1.05, 1.61, 2.48, 3.82, 5.88mg/L, which measured 1.02, 1.84, 2.63, 4.26 and 6.67mg/L, respectively.
Control/dilution water was EPA Duluth laboratory water. Twenty fish were tested per treatment and control. Tank volume = 2L. Control and treatment solution flow rate was equivalent to 18 chamber volumes per day.
Mean test parameters were as follows: temperature = 24.4 deg. C; dissolved oxygen = 7.5 mg/L; pH = 7.8; fish age = 30 days; fish mean wt. = 0.09 g; fish mean length = 18.9 mm; fish loading = 0.0.90 g/L. Organism supplier was U.S. EPA Environmental Research Lab, Duluth, MN, USA.

Reliability : (2) valid with restrictions

18.01.2002 (41)

Type	:	static
Species	:	Carassius auratus (Fish, fresh water)
Exposure period	:	24 hour(s)
Unit	:	mg/l
LC50	:	= 4300 measured/nominal
Limit test	:	
Analytical monitoring	:	yes
Method	:	other: APHA (American Public Health Association) Standard Methods
Year	:	
GLP	:	no data
Test substance	:	

Method	:	Interpolation from a graph of log concentration values versus percent mortality (APHA, 1971).
Remark	:	Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.
Source	:	ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
Test condition	:	A series of treatment solutions were prepared, but their concentrations were not reported. Ten fish were tested per treatment. Tank volume = 25L. Treatment solutions were aerated during the test. Treatment concentrations were analytically verified at test start and termination, but the method of analysis was not reported. Reported results were not distinguished as being based on nominal or measured values and there is no control information. Test parameters were as follows: temperature = 20+/-1 deg. C; dissolved oxygen did not fall below 4 mg/L; initial pH = 7.0; fish average wt. = 3.3+/-1.0 g; fish average length = 6.2+/-0.7 cm.
Reliability	:	(2) valid with restrictions It is unclear from the article as to whether the reported result is based on nominal or measured values. This lack of information, in conjunction with the absence of selected test parameters and results (i.e,, exposure concentrations, mortality), supports a reliability rating of 2. The reported value in this study is comparable to a reported fathead minnow acute value for sBA: 24-hour LC50 = ~4,000 mg/L (Geiger D.L. et al. 1986. Acute Toxicities of Organic Chemicals to Fathead Minnows (Pimephales promelas), Vol. 3. Center for Lake Superior Environmental Studies. University of Wisconsin-Superior, WS, USA.).

17.01.2002 (7)

Type	:	static
Species	:	Leuciscus idus (Fish, fresh water)
Exposure period	:	48 hour(s)
Unit	:	mg/l
LC50	:	= 3520 measured/nominal
Limit test	:	
Analytical monitoring	:	no
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	

Remark	:	Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.
Source	:	EXXON CHEMICAL, Limited Fareham, Hampshire ExxonMobil Biomedical Sciences, Inc., New Jersey, USA EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

17.01.2002 (55)

Type	:	static
Species	:	Petromyzon marinus
Exposure period	:	24 hour(s)
Unit	:	
Limit test	:	
Analytical monitoring	:	no
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	

Method	:	Water used in the study came from Hammond Bay of Lake Huron and taken from a point source that was located 250 feet offshore at a depth of approximately nine feet. Test systems were 10L glass jars that contained 5L of lake water. Test systems were aerated. Up to six organisms were

added to each test system. Larval lampreys (Petromyzon marinus) were collected by means of an electric shocker in the Ocqueoc River, Presque Isle County, Michigan, USA, and were held in running water in aquaria and samll "races" under conditions which simulated their natrual stream habitat.

Water pH ranged from 7.5 to 8.2; water temperature was 55+/-1 degrees F; dissolved oxygen ranged from 8.6 to 13.7 ppm; and free CO2 ranged from 5.0 to 9.0 ppm. Treatment solutions used were 5.0, 1.0, and 0.1 ppm. A control system that only contained lake water was included. It was not stated whether the units were presented as a volume or weight.

Remark : Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.
Result : The highest treatment level tested was 5 ppm. No effects were observed at this level to laral lamprey.
Source : EXXON CHEMICAL, Limited Fareham, Hampshire
ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

18.01.2002 (4)

Type :
Species : other: fish
Exposure period : 96 hour(s)
Unit : mg/l
LC50 : = 1113 calculated
Method : other: ECOSAR Computer Model
Year :
GLP :
Test substance :

Remark : Test Type: Acute Fish Toxicity Calculation
Source : ExxonMobil Biomedical Sciences, Inc., NJ, USA
Test condition : A log Kow (octanol/water partition coefficient) value and a chemical structure are needed to complete the calculation with this model. The log Kow value used was 0.61. The SMILES (Simplified Molecular Input Line Entry System) structure used with the model was: OC(CC)C. Additional data calculated by the model include molecular weight , 74.12, and water solubility, 8,625 mg/L (@25C).
The reference for log Kow is: Hansch, C., A. Leo, and D. Hoekman. 1995. Exploring QSAR - Hydrophobic, Electronic, and Steric Constants. American Chemical Society. Washington, DC, USA.
Reliability : (2) valid with restrictions
Rated 2 for reliability due to calculated value.

17.01.2002 (18)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : static
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
EC50 : = 4227 measured/nominal
Analytical monitoring : no
Method : other: German Institute of Standardization, DIN 38412, Part II, Daphnia Short-Time Test
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Method : None applied. The EC50 was calculated arithmetically from the concentration/effect ratio.

The test method used in this study is similar to the OECD 202 test guideline.

Remark : Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.

Result : 48-hour EC50 = 4,227 mg/L (95% CI 1,859 to 7,143) based on nominal values
The authors considered the test valid because fewer than 10% of the organisms in the control were immobile, the pH value was not below 7.0, and the DO was not below 4.0 mg/L at test termination.

Source : ExxonMobil Biomedical Sciences, Inc., New Jersey, USA

Test condition : The test procedure used daphnids 6 to 24 hours old. Organisms were not fed during the test. The treatment medium was defined and had a total hardness of 2.4 mmol/L, a calcium to magnesium ratio of 4:1, a sodium to potassium ratio of 10:1, and an initial pH value of 8.0+/-0.2. The test solution temperature was 20ºC.
The test systems used 50 ml beakers. Treatment solutions and controls were prepared in duplicate. The organism loading rate was no less than one animal per 2 ml test medium. 20 organisms were tested per treatment and control. Treatment solutions were prepared from a stock sBA solution. Dissolved oxygen (DO) and pH were measured at test termination although specific values were not supplied for this test.

Reliability : (2) valid with restrictions
Although the method was described in the article, data were not provided on the test parameters or results from individual treatment and control solutions. This lack of information supports a reliability rating of 2.

18.01.2002 (58)

Type : static
Species : Daphnia magna (Crustacea)
Exposure period : 24 hour(s)
Unit : mg/l
LC50 : = 3750 measured/nominal
Analytical monitoring : no
Method : other: not specified
Year :
GLP : no data
Test substance :

Remark : Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.

Source : EXXON CHEMICAL, Limited Fareham, Hampshire
ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

17.01.2002 (9)

Type : static
Species : other: Tetrahymena pyrifomis (Ciliate)
Exposure period : 48 hour(s)
Unit : mg/l
EC50 : = 3196 measured/nominal
Analytical monitoring : no data
Method : other: Population Growth Impairment Test
Year :
GLP : no data
Test substance :

Method : Probit analysis procedure using Statistical Analysis System (SAS) software (SAS Institute, 1989).

Remark : Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.

Result : 48-hour EC50 for growth = 3,196 mg/L based on nominal values
Population density (growth) was measured spectrophotometrically as

absorbance at 540 nm.

Source	:	ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
Test condition	:	Axenic cultures of Tetrahymena pyrifomis were used in the test. Only 48-hour population densities were measured. Treatment solutions and controls were prepared in duplicate. Treatment solutions were prepared from a stock sBA solution.
Reliability	:	(2) valid with restrictions A non-standardized method was referenced in the article. Data were not provided on the test parameters or results from individual treatment and control solutions. This lack of information supports a reliability rating of 2.

17.01.2002 (79)

Type	:	
Species	:	other: Daphnid
Exposure period	:	48 hour(s)
Unit	:	mg/l
LC50	:	= 1084 calculated
Method	:	other: ECOSAR Computer Model
Year	:	
GLP	:	
Test substance	:	

Remark	:	Test Type: Acute Daphnid Toxicity Calculation
Source	:	ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
Test condition	:	A log Kow (octanol/water partition coefficient) value and a chemical structure are needed to complete the calculation with this model. The log Kow value used was 0.61. The SMILES (Simplified Molecular Input Line Entry System) structure used with the model was: OC(CC)C. Additional data calculated by the model include molecular weight , 74.12, and water solubility, 8,625 mg/L (@25C). The reference for log Kow is: Hansch, C., A. Leo, and D. Hoekman. 1995. Exploring QSAR - Hydrophobic, Electronic, and Steric Constants. American Chemical Society. Washington, DC, USA.
Reliability	:	(2) valid with restrictions Rated 2 for reliability due to calculated value.

17.01.2002 (18)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	Scenedesmus quadricauda (Algae)
Endpoint	:	
Exposure period	:	7 day(s)
Unit	:	mg/l
TT	:	= 95 measured/nominal
Limit test	:	
Analytical monitoring	:	no
Method	:	other: 7-Day Cell Multiplication Inhibition Test
Year	:	
GLP	:	no data
Test substance	:	

Method	:	None applied. The toxicity threshold (TT) was determined graphically by plotting the highest non-toxic concentration versus its mean extinction value against the lowest toxic concentration versus its mean extinction value and calculating the toxicant concentration at 3% below the no effect level.
Remark	:	Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%. Test Type: Static Toxicity Test
Result	:	7-day TT (toxicity threshold) for growth = 95 mg/L based on nominal

values.
The TT value for growth is calculated by identifying the treatment level that is greater or equal to 3% below the treatment level that did not exhibit toxic effects as measured by the extinction of primary light of monochromatic radiation at 578 nm.

Source : ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
Test condition : Treatment solutions were prepared by diluting a stock sBA solution. Testing was conducted in metal capped, 300 ml Erlenmeyer flasks containing 50 ml of treatment solution. Treatment solutions contained sBA, cells, double distilled water, and a sterile, defined nutrient medium. The control solution contained nutrient medium, to which sterile double distilled water was added. Growth inhibition measurements were only determined on day 7.
Cell growth was determined by using a turbidimetric procedure that measured primary light extinction (monochromatic radiation at 578 nm) through a cell suspension of 10 mm thickness.
Reliability : (2) valid with restrictions
Although a non-standardized method was described in the article, data were not provided on the test parameters, replication, or results from individual treatment and control solutions. This lack of information supports a reliability rating of 2.

17.01.2002 (13)

Species : other algae: green alga
Endpoint :
Exposure period : 96 hour(s)
Unit : mg/l
EC50 : = 625 calculated
Method : other: ECOSAR Computer Model
Year :
GLP :
Test substance :

Remark : Test Type: Green Alga Toxicity Calculation
Result : 96-hour EC50 = 625 mg/L
Source : ExxonMobil Biomedical Sciences, Inc., NJ, USA
Test condition : A log Kow (octanol/water partition coefficient) value and a chemical structure are needed to complete the calculation with this model. The log Kow value used was 0.61. The SMILES (Simplified Molecular Input Line Entry System) structure used with the model was: OC(CC)C. Additional data calculated by the model include molecular weight , 74.12, and water solubility, 8,625 mg/L (@25C).
The reference for log Kow is: Hansch, C., A. Leo, and D. Hoekman. 1995. Exploring QSAR - Hydrophobic, Electronic, and Steric Constants. American Chemical Society. Washington, DC, USA.
Reliability : (2) valid with restrictions
Rated 2 for reliability due to calculated value.

17.01.2002 (18)

Species :
Endpoint : other: green alga
Exposure period : 96 hour(s)
Unit : mg/l
ChV* : = 28 calculated
Method : other: ECOSAR Computer Model
Year :
GLP :
Test substance :

Result : *Chronic value
Source : ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
Test condition : A log Kow (octanol/water partition coefficient) value and a chemical

structure are needed to complete the calculation with this model. The log Kow value used was 0.61. The SMILES (Simplified Molecular Input Line Entry System) structure used with the model was: OC(CC)C. Additional data calculated by the model include molecular weight , 74.12, and water solubility, 8,625 mg/L (@25C).
The reference for log Kow is: Hansch, C., A. Leo, and D. Hoekman. 1995. Exploring QSAR - Hydrophobic, Electronic, and Steric Constants. American Chemical Society. Washington, DC, USA.

Reliability : (2) valid with restrictions
Rated 2 for reliability due to calculated value.

18.01.2002 (18)

Species	:	Microcystis aeruginosa (Algae, blue, cyanobacteria)
Endpoint	:	
Exposure period	:	192 hour(s)
Unit	:	mg/l
NOEC	:	= 312 measured/nominal
Limit test	:	
Analytical monitoring	:	no data
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	

Remark : Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.

Source : ExxonMobil Biomedical Sciences, Inc., New Jersey, USA

18.01.2002 (8)

Species	:	Chlorella pyrenoidosa (Algae)
Endpoint	:	
Exposure period	:	
Unit	:	mg/l
NOEC	:	= 8900 measured/nominal
Limit test	:	
Analytical monitoring	:	no data
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	

Remark : Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.

Source : ExxonMobil Biomedical Sciences, Inc., New Jersey, USA

18.01.2002 (54)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

Type	:	aquatic
Species	:	Pseudomonas putida (Bacteria)
Exposure period	:	16 hour(s)
Unit	:	mg/l
EC0	:	ca. 500 measured/nominal
NOAEL	:	= 500
Analytical monitoring	:	no data
Method	:	other: total biomass
Year	:	
GLP	:	no data
Test substance	:	

Remark	:	Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.
Source	:	ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
18.01.2002		(12)

Type	:	
Species	:	Bacillus subtilis (Bacteria)
Exposure period	:	
Unit	:	mg/l
EC50	:	= 1630 measured/nominal
Analytical monitoring	:	no data
Method	:	
Year	:	
GLP	:	no data
Test substance	:	

Source	:	EXXON CHEMICAL, Limited Fareham, Hampshire ExxonMobil Biomedical Sciences, Inc., New Jersey, USA EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
18.01.2002		(36)

Type	:	aquatic
Species	:	Chilomonas paramaecium (Protozoa)
Exposure period	:	48 hour(s)
Unit	:	mg/l
NOEL	:	= 745 measured/nominal
Analytical monitoring	:	no data
Method	:	other: total biomass
Year	:	
GLP	:	no data
Test substance	:	

Remark	:	Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.
Source	:	EXXON CHEMICAL, Limited Fareham, Hampshire ExxonMobil Biomedical Sciences, Inc., New Jersey, USA EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
18.01.2002		

Type	:	aquatic
Species	:	Entosiphon sulcatum (Protozoa)
Exposure period	:	72 hour(s)
Unit	:	mg/l
NOEL	:	= 1282 measured/nominal
Analytical monitoring	:	no data
Method	:	other: total biomass
Year	:	
GLP	:	no data
Test substance	:	

Remark	:	Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.
Source	:	ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
18.01.2002		(11)

Type	:	aquatic
Species	:	Uronema parduzci (Protozoa)
Exposure period	:	20 hour(s)
Unit	:	mg/l
NOEC	:	= 1416
Analytical monitoring	:	no data
Method	:	other: total biomass

Year	:	
GLP	:	no data
Test substance	:	
Remark	:	Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.
Source	:	ExxonMobil Biomedical Sciences, Inc., New Jersey, USA

17.01.2002 (10)

4.5.1 CHRONIC TOXICITY TO FISH

Species	:	other: fish
Endpoint	:	
Exposure period	:	30 day(s)
Unit	:	mg/l
ChV*	:	= 115 calculated
Method	:	other: ECOSAR Computer Model
Year	:	
GLP	:	
Test substance	:	
Remark	:	Test Type: Chronic Fish Toxicity Calculation * Chronic Value
Source	:	ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
Test condition	:	A log Kow (octanol/water partition coefficient) value and a chemical structure are needed to complete the calculation with this model. The log Kow value used was 0.61. The SMILES (Simplified Molecular Input Line Entry System) structure used with the model was: OC(CC)C. Additional data calculated by the model include molecular weight , 74.12, and water solubility, 8,625 mg/L (@25C). The reference for log Kow is: Hansch, C., A. Leo, and D. Hoekman. 1995. Exploring QSAR - Hydrophobic, Electronic, and Steric Constants. American Chemical Society. Washington, DC, USA.
Reliability	:	(2) valid with restrictions Rated 2 for reliability due to calculated value.

17.01.2002 (18)

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

Species	:	other: Daphnid
Endpoint	:	
Exposure period	:	16 day(s)
Unit	:	mg/l
EC50	:	= 30 calculated
Method	:	other: ECOSAR Computer Model
Year	:	
GLP	:	
Test substance	:	
Remark	:	Test Type: Chronic Daphnid Toxicity Calculation
Source	:	ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
Test condition	:	A log Kow (octanol/water partition coefficient) value and a chemical structure are needed to complete the calculation with this model. The log Kow value used was 0.61. The SMILES (Simplified Molecular Input Line Entry System) structure used with the model was: OC(CC)C. Additional data calculated by the model include molecular weight , 74.12, and water solubility, 8,625 mg/L (@25C). The reference for log Kow is: Hansch, C., A. Leo, and D. Hoekman. 1995.

Exploring QSAR - Hydrophobic, Electronic, and Steric Constants. American Chemical Society. Washington, DC, USA.

Reliability : (2) valid with restrictions
Rated 2 for reliability due to calculated value.

17.01.2002 (18)

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

Species : other terrestrial plant: Solanum tuberosum L.
Endpoint :
Exposure period :
Unit :
Method :
Year :
GLP : no data
Test substance :

Method : stage at application: seedling, on intact plant, in environmental chamber, application by fumigation: 2 cm3/l.
Remark : Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.
Result : 20% respiration increase, on tuber
Source : EXXON CHEMICAL, Limited Fareham, Hampshire
ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

17.01.2002 (66)

Species : other terrestrial plant: wheat
Endpoint :
Exposure period :
Unit :
Method :
Year :
GLP : no data
Test substance :

Method : Stage at application: seedling, on excised organ; addition to growth medium, dose: 4 x 10E-2 M
Remark : Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.
Result : 50% decrease in number of cells
Source : EXXON CHEMICAL, Limited Fareham, Hampshire
ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

17.01.2002 (45)

Species : other terrestrial plant: wheat
Endpoint :
Exposure period :
Unit :
Method :
Year :
GLP : no data
Test substance :

Method : Stage at application: seedling, on excised organ; addition

to growth medium, dose: 5 x 10 E-2 M.

Remark	:	Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.
Result	:	50% size decrease of cells
Source	:	EXXON CHEMICAL, Limited Fareham, Hampshire ExxonMobil Biomedical Sciences, Inc., New Jersey, USA EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

17.01.2002 (44)

Species	:	other terrestrial plant: Lupinus albus
Endpoint	:	
Exposure period	:	1 day(s)
Unit	:	
Method	:	
Year	:	
GLP	:	no data
Test substance	:	
Method	:	Stage at application: seedling, on intact plant; addition to growth meduim, in culture flask, dose = 1%.
Remark	:	Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.
Result	:	73% size decrease of root
Source	:	EXXON CHEMICAL, Limited Fareham, Hampshire ExxonMobil Biomedical Sciences, Inc., New Jersey, USA EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

17.01.2002 (63)

Species	:	Lactuca sativa (Dicotyledon)
Endpoint	:	other: seed germination
Exposure period	:	
Unit	:	mg/l
EC50	:	= 650
Method	:	other: not indicated
Year	:	
GLP	:	no data
Test substance	:	
Remark	:	Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.
Source	:	EXXON CHEMICAL, Limited Fareham, Hampshire ExxonMobil Biomedical Sciences, Inc., New Jersey, USA EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

17.01.2002 (91)

Species	:	other terrestrial plant: Cucumis sativus
Endpoint	:	other: seed germination
Exposure period	:	
Unit	:	mg/l
NOEC	:	< 50375
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	
Remark	:	Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.
Source	:	EXXON CHEMICAL, Limited Fareham, Hampshire ExxonMobil Biomedical Sciences, Inc., New Jersey, USA EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

17.01.2002 (91)

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

Type	:	
Species	:	other: earthworm
Endpoint	:	mortality
Exposure period	:	14 day(s)
Unit	:	other: ppm
LC50	:	= 1222 calculated
Method	:	other: ECOSAR Computer Model
Year	:	
GLP	:	
Test substance	:	
Remark	:	Test Type: Earthworm Toxicity Calculation
Source	:	ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
Test condition	:	A log Kow (octanol/water partition coefficient) value and a chemical structure are needed to complete the calculation with this model. The log Kow value used was 0.61. The SMILES (Simplified Molecular Input Line Entry System) structure used with the model was: OC(CC)C. Additional data calculated by the model include molecular weight , 74.12, and water solubility, 8,625 mg/L (@25C). The reference for log Kow is: Hansch, C., A. Leo, and D. Hoekman. 1995. Exploring QSAR - Hydrophobic, Electronic, and Steric Constants. American Chemical Society. Washington, DC, USA.
Reliability	:	(2) valid with restrictions Rated 2 for reliability due to calculated value.

17.01.2002 (18)

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

Species	:	other: Xenopus laevis (Clawed Frog)
Endpoint	:	mortality
Exposure period	:	48 hour(s)
Unit	:	other: mg/L
LC50	:	= 1530 measured/nominal
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	
Method	:	Median lethal concentration was calculated as a projection from the least square linear regression on log transformed nominal concentration data and probit transformed percent effect data.
Remark	:	Test Type: Static Acute Toxicity Test Analytical Monitoring: No Results based on nominal treatment values. Information on sBA purity is not available; assumed to have used a commercial grade of >/= 99%.
Source	:	ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
Test condition	:	The test procedure used 3 to 4 week old larvae. The organisms were exposed in covered all-glass aquaria containing 1L of Dutch Standard Water at a temperature of 20+/-1C. The test material was added once at the beginning of the study. Five concentration levels were evaluated with 10 organisms per level. The 5 levels had a factorial difference of 1.5. Mortality was only recorded after 48 hours. The test species, Xenopus laevis, was identified in the article as a clawed toad. However, it is correctly identified as a clawed frog in this robust summary.
Reliability	:	(2) valid with restrictions

The test procedure was generally described in the article. Data were not provided on the test parameters or results from individual treatment and control solutions. This lack of information supports a reliability rating of 2.

18.01.2002 (24)

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

In Vitro/in vivo	:	
Type	:	
Species	:	rat
Number of animals		
Males	:	
Females	:	
Doses		
Males	:	(See Remark)
Females	:	
Vehicle	:	other: Aqueous Solution
Route of administration	:	other: Oral Gavage / i.v.
Exposure time	:	
Product type guidance	:	
Decision on results on acute tox. tests	:	
Adverse effects on prolonged exposure	:	
Half-lives	:	1st: 2nd: 3rd:
Toxic behaviour	:	
Deg. product	:	
Method	:	other: Experimental Model Development
Year	:	1981
GLP	:	no data
Test substance	:	other TS: 2-Butanol (sec-Butanol; sBA) and metabolites 2-Butanone (Methyl ethyl ketone; MEK), 3-Hydroxy-2-Butanone (3H-2B), and 2,3-Butanediol (2,3-BD) (CAS Nos. 78-92-2 (sBA); 78-93-3 (MEK))
Method	:	Statistical Methods Student's t-test was used for statistical evaluation of differences between two means. In the pharmacokinetic model, the differential equations were solved numerically by a Hammings Predictor-Correction method with a Runge-Kutta starter.
Remark	:	Dietz et al. (1981) selected doses for MEK and sBA based on the earlier pharmacokinetic analysis (Traiger and Bruckner, 1976) that established approximately 96% of an administered dose of sBA was oxidized in vivo to MEK. Thus 1960 mg/kg (2.1 ml/kg) of MEK estimates the amount of MEK formed in vivo from a dose of 1776 mg/kg (2.2 ml/kg) of sBA. Male rats were given oral doses of sBA, MEK, 2-3 B-D (or i.v.), or 3H-2B (i.v.) and serial blood samples were collected for up to 30 hours following treatment. Test Type: Metabolism and Pharmacokinetic Evaluation Strain: Sprague-Dawley Dose Groups/Concentrations: sBA: 2.2 ml/kg or 1776 mg/kg as a 22% aqueous solution (oral). MEK: 2.1ml/kg or 1690 mg/kg as a 21% aqueous solution (oral). 2,3-BD : 0.68 ml/kg or 676 mg/kg as a 6.8 % aqueous solution (oral or i.v.). 3H-2B: 400 or 800 mg/kg as a 60% aqueous solution (i.v.) Frequency of Treatment: Single Dose (oral or i.v.) Duration of Test: 30 Hours Sex: Male Number/Dose Group: Not Identified
Result	:	In the sBA-treatment phase of the study, blood concentrations of sBA and its metabolites MEK, 3H-2B, and 2,3-BD were measured. Blood sBA concentrations of 0.59 mg/ml peaked at 2 hours and declined to less than 0.05 mg/ml at 16 hours. As the sBA concentration fell, the metabolite concentrations of MEK, 3H-2B, and 2,3-BD concentrations rose to maximums at 8, 12, and 18hr, respectively. The peak concentration of MEK was 0.78 mg/ml, while that of 2,3-BD was 0.21 mg/ml. 3H-2B reached a

peak concentration of 0.04 mg/ml. Total AUC values for sBA, MEK, 3H-2B, and 2,3-BD were 3254 ± 258, 9868 ± 566, 443 ± 93, and 3167 ± 503 mg-hr/l, respectively.
Following an oral dose of MEK, blood concentrations of MEK and its metabolites sBA, 3H-2B, and 2,3-BD were measured. Blood MEK concentrations of 0.95 mg/ml peaked at 4 hours and declined to less than 0.07 mg/ml at 18 hours. As the MEK concentration fell, the end metabolite 2,3-BD rose to a maximum concentration of 0.26 mg/ml at 18 hours. Peak concentrations of sBA and 3H-2B were 0.033 and 0.027 mg/ml, respectively. These were detected at 6 and 8 hr after the MEK administration. Total AUC values for MEK, sBA, 3H-2B, and 2,3-BD were 10,899 ± 824, 414 ± 38, 382 ± 38, and 3863 ± 238 mg-hr/l, respectively.

Test substance : 2-Butanol (sec-Butanol; sBA) and metabolites 2-Butanone (Methyl ethyl ketone; MEK), 3-Hydroxy-2-Butanone (3H-2B), and 2,3-Butanediol (2,3-BD) (CAS Nos. 78-92-2 (sBA); 78-93-3 (MEK))
Purity not identified.

Conclusion : In the development of the model, the authors confirmed that a limited amount of sBA could be recovered as glucuronide in the urine. Most of the alcohol appears to undergo oxidation via alcohol dehydrogenase to its corresponding ketone, MEK. The results showed a limited amount of the ketone undergoes a backward reduction to its parent alcohol, sBA. 3H-2B and 2,3-BD are found to be common metabolites of sBA and MEK. The model was able to simulate blood concentrations and elimination of all 4 compounds after oral administration of sBA, and the results after i.v. of 3H-2B and 2,3-BD. AUC analysis suggested that the quantities of 3H-2B and 2,3-BD formed from oral doses of sBA and MEK are comparable. The results supported the estimation in that no significant difference in the AUC of MEK was observed after dosing with either 1776 mg/kg of sBA or 1690 mg/kg of MEK (10,899 ± 824 vs. 9868 ± 566 mg-hr /liter, respectively).

Reliability : (1) valid without restriction
No circumstances occurred that would have affected the quality or integrity of the data. Test procedures were in accordance with generally accepted scientific standards and described in sufficient detail.

01.06.2006 (25)

In Vitro/in vivo :
Type :
Species : guinea pig
Number of animals
Males :
Females :
Doses
Males : 450 mg/kg body weight
Females :
Vehicle : other: Corn oil (25% solution)
Route of administration : i.p.
Exposure time :
Product type guidance :
Decision on results on acute tox. tests :
Adverse effects on prolonged exposure :
Half-lives : 1st.:
2nd.:
3rd.:
Toxic behaviour :
Deg. product :
Method : other: Experimental
Year : 1976
GLP : no data
Test substance : other TS: 2-Butanone (Methyl ethyl ketone; MEK) (CAS No. 78-93-3)

Remark : Male guinea pigs ranging in weight from 250 - 450 grams were given a single i.p. dose of 450mg/kg MEK (study also investigated MnBK and MiBK

- data not addressed here). Blood was collected by heart puncture from 4 animals at each of the following times after dose administration: 1, 2, 4, 6, 8, 12, and 16 Hr. Only 1 sample was collected from each guinea pig. Serum was separated and refrigerated until assayed within 48 Hr. The concentrations of the ketones and their metabolites were measured in duplicate by direct on-column injection of undiluted serum into a Varian 2100 Gas Chromatograph equipped with a flame ionization detector. Ketones and metabolites were quantitated from calibration curves prepared from pure standards. Greater than 90% of each ketone was distributed in the plasma fraction. Half-lives were estimated by extrapolating the linear portion of the decay curve to zero time.
Test Type: Metabolism and Pharmacokinetic Evaluation
Frequency of Treatment: Single injection
Duration of Test: 16 Hours
Number/Dose Group: 4 at each blood - sampling interval

Result : MEK: 2-Butanol, 3-hydroxy-2-butanone, and 2,3-butanediol were identified as metabolites in the serum of guinea pigs injected i.p. with MEK. The half-life of MEK in serum was 270 min. The clearance time of MEK was 12 Hr. 2,3-Butanediol was cleared in 16 hours, as were the other two metabolites. The metabolism was described as oxidation via hydroxylation of the ? -1 carbon forming 3-hydroxy-2-butanone as the metabolite of MEK. Reduction occurred at the carbonyl group as expected forming the secondary alcohol, 2-butanol from MEK.

Test substance : 2-Butanone (Methyl ethyl ketone; MEK) (CAS No. 78-93-3)
Purity: 98% with traces of 2-butanol

Conclusion : This study showed the initial metabolism of MEK follows both oxidative and reductive pathways to produce 3-hydroxy-2-butanone, 2,3-butanediol and 2-butanol.

Reliability : (1) valid without restriction
No circumstances occurred that would have affected the quality or integrity of the data. Test procedures were in accordance with generally accepted scientific standards and described in sufficient detail.

01.06.2006 (27)

In Vitro/in vivo :
Type :
Species : human
Number of animals
Males : 9
Females :
Doses
Males : 200 ppm (8.2mmol/m3)
Females :
Vehicle : other: none
Route of administration : inhalation
Exposure time :
Product type guidance :
Decision on results on acute tox. tests :
Adverse effects on prolonged exposure :
Half-lives : 1st.:
2nd.:
3rd.:
Toxic behaviour :
Deg. product :
Method : other: Experimental
Year : 1988
GLP : no data
Test substance : other TS: 2-Butanone (Methyl ethyl ketone; MEK) (CAS No. 78-93-3)

Remark : Nine healthy male volunteers, 18-34 years of age (mean 23.7), weight 65-81 kg (mean 74.3), height 172-190 cm (mean 181.8) and calculated surface area 1.81 - 2.09 m2 (mean 1.97) were exposed for 4 Hr to 200ppm

MEK on 2 separate days at least 1 week apart. Venous blood samples were collected at 1-hr intervals during exposure and over 120 to 210 minutes post-exposure. In a supplementary study, follow-up elimination blood samples were collected in 2 persons until the next morning. One of the exposures constituted sedentary activity and the other encompassed three 100 W ergometric exercise periods over minutes 5-15, 95-105 and 225-235 during a total exposure of 240 minutes. Exhaled air samples were collected with a 2-way respirator mouthpiece into 4-liter polyester laminated aluminum-foil bags and analyzed immediately. Samples were collected at one-hour intervals during exposure and over 120-210 minutes thereafter. Urine samples were obtained at 2-hour intervals during the exposure day and in separate samples until the next morning. Whole venous blood was analyzed by gas chromatography, as were air samples. Peaks were compared to calibration curves prepared of known blood or air concentrations of MEK. 2-3BD in urine was analyzed according to a modification of the method of Robinson and Reive. The 2 peaks in the chromatograph (d,l-forms and meso-form) were summed for calculations.
Test Type: Metabolism and Pharmacokinetic Evaluation
Frequency of Treatment: 2 Exposure periods at least 1 wk between
Duration of Test: 4 Hr. Exposure

Result : Pulmonary retention of MEK in the lungs remained constant throughout exposure with or without exercise. Relative uptake was 53% ± 2%. Estimated mean total pulmonary uptakes were 11.4 mmol (ventilation volume 11 liters/min at rest) and 14.3 mmol (ventilation volume 35 liters/min during the exercise). Blood MEK concentrations increased rapidly during the first hour of exposure (markedly faster when associated with exercise). Thereafter, concentrations increased slowly and linearly through 4 hr with sedentary activity and steeply during the exercise period at the end of the 4 hr exposure period. Two elimination phases were detected for MEK in blood. The calculated half-time for the faster phase of elimination (0-45 min post-exposure) was 30 min and about 81 min for the slower phase (60-320 min post-exposure). Owing to remarkable solubility of MEK, only 2-3% of absorbed dose was eliminated by exhalation. Urinary excretion of unchanged MEK was 0.1% and excretion of the metabolite 2H3B was about 0.1%. The authors speculated that the greater part of absorbed MEK is probably converted to products of intermediary metabolism, e.g., to acetate or acetoacetate via 3H2B.

Test substance : 2-Butanone (Methyl ethyl ketone; MEK) (CAS No. 78-93-3)
Purity: Analytical Grade

Conclusion : Two elimination phases were detected for MEK in blood. The T½ for the faster phase of elimination was 30 min and about 81 min for the slower phase. 2-3% of absorbed dose of MEK was eliminated by exhalation. Urinary excretion of unchanged MEK was 0.1% and excretion of the metabolite 2H3B was about 0.1%.

Reliability : (1) valid without restriction
No circumstances occurred that would have affected the quality or integrity of the data. Test procedures were in accordance with generally accepted scientific standards and described in sufficient detail.

01.06.2006 (60)

5.1.1 ACUTE ORAL TOXICITY

Type :
Value : = 6500 mg/kg bw
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Doses :

Method	:	other
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	EXXON CHEMICAL, Limited Fareham, Hampshire EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

21.10.1992 (34)

Type	:	LD50
Value	:	= 2054 - 2328 mg/kg bw
Species	:	rat
Strain	:	Fischer 344
Sex	:	male/female
Number of animals	:	10
Vehicle	:	other: None
Doses	:	
Method	:	other: Experimental (Non-regulatory)
Year	:	1986
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Fischer 344 rats were in the age range of 55-65 days when purchased and were 9 -11 weeks old when the study commenced. All animals were fasted for 18 hours prior to dosing and doses were altered by varying the volume dispensed from the syringe. Body weights were recorded on Days 1, 7 and 14. All surviving rats gained weight by the end of the 14-day observation period. The LD50's were calculated using probit analysis Route of Administration: Oral Gavage Doses: 950 - 2400 mg/kg Volume Administered: Single dose volume varied by body weight Post Dose Observation Period: Daily for 14 Days Purity: 99.5%
Result	:	2054 mg/kg (95% fiducial limits, 1283 - 4018 mg/kg) males, 2328 mg/kg (95% fiducial limits, 1470 - 5428 mg/kg) females, and 2193 mg/kg (95% fiducial limits, 1608 - 4146 mg/kg) combined.
Conclusion	:	The acute oral LD50 for sBA in Fischer 344 rats is 2193 mg/kg.
Reliability	:	(1) valid without restriction 1 - Reliable study without restrictions. No circumstances occurred that would have affected the quality or integrity of the data.

10.01.2002 (72)

Type	:	LD50
Value	:	= 5730 - 7320 mg/kg bw
Species	:	rat
Strain	:	other: Carworth-Wistar
Sex	:	male
Number of animals	:	5
Vehicle	:	other: Unknown (water, corn oil, or a 1% solution of 3,9-diethyl-6-tridecanol sulfate (Tergitol Penetrant 7)
Doses	:	
Method	:	other: Experimental (Non-regulatory)
Year	:	1954
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Route of Administration: Oral Gavage Doses: Logarithmic series Dose Volume Administered: Single dose; 1-10 ml/rat Post Dose Observation Period: 14 Days The animals weighed 90 - 120 grams and were not fasted prior to dosing. The most probable LD50 value and the fiducial range were estimated by

the method of Thompson using the tables of Weil.

Result	:	6.48 g/kg (5.73 - 7.32)
Conclusion	:	The acute oral LD50 for sBA in Carworth-Wistar rats is 6.48 g/kg (5.73 - 7.32)
Reliability	:	(2) valid with restrictions Smyth, H. F. Jr., Carpenter, C. P., Weil, C. S., and Pozzani, U. C. (1954). Range-finding toxicity data: List V. Arch Ind Hyg Occup Med, 10:61-68.

10.01.2002 (83)

Type	:	LD50
Value	:	= 4900 mg/kg bw
Species	:	rabbit
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	other: not specified
Year	:	1972
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	EXXON CHEMICAL, Limited Fareham, Hampshire EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

21.10.1992

Type	:	LD50
Value	:	= 4890 mg/kg bw
Species	:	rabbit
Strain	:	other: Unknown
Sex	:	male/female
Number of animals	:	
Vehicle	:	no data
Doses	:	
Method	:	other: Experimental (Non-regulatory)
Year	:	1925
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Route of Administration: Oral Gavage Number of Animals/Dose: Unknown Doses: 14 or 66 mmol/kg; 1037 or 4890 mg/kg Dose Volume Administered: < 50 ml Post Dose Observation Period: 24 Hours Ten to 35 rabbits weighing between 1.5 and 2.5 kg were given "calculated" quantities of sBA at doses described as the "Narcotic Dose " or "Certain Lethal Dose" by oral gavage and observed for 24 hours. The cited LD50 [66 mmol/kg, or 4890 mg/kg] is really the Certain Lethal Dose presented in the paper by Munch and Schwartze (1925). The Munch paper (1972) presents the rabbit data reported earlier in 1925 plus tadpole data. Because of the inconsistency in the definition of LD50 and Certain Lethal Dose, a CoR of 3 is assigned to both references.
Result	:	4890 mg/kg
Conclusion	:	The reported LD50 was 66 mmol/kg (4890 mg/kg).
Reliability	:	(3) invalid 3 - Not Reliable. Study is pre-GLP and documentation insufficient for assessment

10.01.2002 (67) (68)

5.1.2 ACUTE INHALATION TOXICITY

Type	:	LC50
Value	:	= 16000 ppm
Species	:	rat
Strain	:	other: Carworth-Wistar
Sex	:	male
Number of animals	:	6
Vehicle	:	other: None
Doses	:	
Exposure time	:	4 hour(s)
Method	:	other: Experimental (Non-regulatory)
Year	:	1954
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Route of Administration: Inhalation Observation Period: Up to 14 days The study consisted of exposing six male albino rats to a flowing stream of air approaching saturation with sBA vapors. The stream was prepared by proportioning pumps and nominal concentrations (not confirmed by analytical methods) were recorded. The study end point was the concentration yielding a fractional mortality among six rats within 14 days.
Result	:	16,000 ppm sBA was lethal to 5 of 6 rats within 14 days
Source	:	EXXON CHEMICAL, Limited Fareham, Hampshire EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Conclusion	:	Five of six exposed rats died within 14 days.
Reliability	:	(2) valid with restrictions 2- Reliable with restrictions. Pre-GLP study documented, meets generally accepted scientific principles, acceptable for assessment.

11.01.2002 (83)

Type	:	LC50
Value	:	= 8000 ppm
Species	:	rat
Strain	:	other: Carworth-Wistar
Sex	:	male
Number of animals	:	6
Vehicle	:	other: None
Doses	:	
Exposure time	:	4 hour(s)
Method	:	other: Experimental (Non-regulatory)
Year	:	1951
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Route of Administration: Inhalation Observation Period: Up to 14 days The study consisted of exposing six male albino rats to a flowing stream of air with sBA vapors. The stream was prepared by proportioning pumps and nominal concentrations (not confirmed by analytical methods) were recorded. The study end point was the concentration yielding a fractional mortality among six rats within 14 days.
Result	:	8,000 ppm sBA was lethal to 1 of 6 rats within 14 days
Conclusion	:	One of six exposed rats died within 14 days.
Reliability	:	(2) valid with restrictions 2- Reliable with restrictions. Pre-GLP study documented, meets generally accepted scientific principles, acceptable for assessment.

10.01.2002 (65)

Type	:	LC50

Value	:	= 10000 ppm
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	female
Number of animals	:	5
Vehicle	:	other: None
Doses	:	
Exposure time	:	7 hour(s)
Method	:	other: Experimental (Non-regulatory)
Year	:	1989
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Study Type: Acute Inhalation (Pilot for Teratology study) Purity: >or= 99 % Route of Administration: Inhalation Observation Period: Unknown The study consisted of exposing five female rats to a flowing stream of air with sBA vapors. The stream was prepared by proportioning pumps. The study end point was the concentration yielding a fractional mortality.
Result	:	10,000 ppm sBA was lethal to 5 of 5 rats
Conclusion	:	Five of five exposed female rats died following a single 7 hour exposure.
Reliability	:	(2) valid with restrictions 2 - Reliable. Pilot study with acceptable restrictions.

10.01.2002 (69)

Type	:	LC50
Value	:	
Species	:	mouse
Strain	:	no data
Sex	:	no data
Number of animals	:	2
Vehicle	:	other: None
Doses	:	
Exposure time	:	
Method	:	other: Experimental (Non-regulatory)
Year	:	1938
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	1650 ppm: no signs of intoxication after 420 minutes. 3300 ppm: ataxia in 51-100 minutes, prostration in 120-180 minutes, narcosis in 3000 minutes, no deaths 19,800 ppm: ataxia in 7-8 minutes, prostration in 12-20 minutes, narcosis in 40 minutes, no deaths Route of Administration: Inhalation Doses/time: 1650, 3300, 19800 ppm/decreasing lengths of time Post Dose Observation Period: Various
Result	:	Not Defined
Conclusion	:	Doses from 3,300 to 19,800 ppm induced narcosis but not death.
Reliability	:	(4) not assignable 4 - Documentation insufficient for assessment. Non-guideline pre-GLP study.

10.01.2002 (85)

5.1.3 ACUTE DERMAL TOXICITY

Type	:	other: Limit
Value	:	> 2000 mg/kg bw
Species	:	rat

Strain	:	Fischer 344
Sex	:	male/female
Number of animals	:	10
Vehicle	:	other: None
Doses	:	
Method	:	other: Experimental (Non-regulatory)
Year	:	1986
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4

Remark : Fischer 344 rats were in the age range of 55-65 days when purchased and were 9 -11 weeks old when the study commenced. The day before dosing the animals, approximately 60% of the dorsal hair was closely shorn with fine electric clippers, and the rats and the rats were weighed on the day of dosing. Varying the volume dispensed from the syringe altered doses. Application was made at room temperature and the test material was covered with aluminum foil and held in place by a double over-wrap of waterproof adhesive tape. The rats were individually housed for the next 24 hours. Food was withheld, but water was available ad libitum. At the end of the 24-hour period, the tape and foil were removed and the skin was washed with warm dilute detergent solution and then dried. The animals were observed for signs of toxicity for 14 days after dosing. Body weights were recorded on Days 1, 7 and 14. None of the rats died. There were no overt signs of toxicity and all rats gained weight relative to their day 1body weight.
Route of Administration: Dermal
Doses/time: 2000 mg/kg single application / 24-hour occlusive patch
Post Dose Observation Period: Daily for 14 Days
Purity: 99.5%

Result	:	> 2000 mg/kg
Conclusion	:	The acute percutaneous LD50 of undiluted sBA in rats was > 2000 mg/kg.
Reliability	:	(1) valid without restriction 1 - Reliable without Restrictions. No circumstances occurred that would have affected the quality or integrity of the data.

10.01.2002 (73)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

Type	:	LD50
Value	:	= 800 mg/kg bw
Species	:	mouse
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Route of admin.	:	i.p.
Exposure time	:	
Method	:	other: not specified
Year	:	1978
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4

Source : EXXON CHEMICAL, Limited Fareham, Hampshire
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

21.10.1992

5.2.1 SKIN IRRITATION

Species	:	rabbit
Concentration	:	
Exposure	:	
Exposure time	:	
Number of animals	:	
Vehicle	:	
PDII	:	
Result	:	not irritating
Classification	:	not irritating
Method	:	other: not specified
Year	:	1954
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4

Source : EXXON CHEMICAL, Limited Fareham, Hampshire
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
21.10.1992 (33)

Species	:	rabbit
Concentration	:	
Exposure	:	Occlusive
Exposure time	:	4 hour(s)
Number of animals	:	6
Vehicle	:	
PDII	:	
Result	:	not irritating
Classification	:	not irritating
Method	:	OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year	:	1986
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4

Remark : New Zealand White rabbits, 3 - 6 months of age, were acclimated to the laboratory conditions for at least 2 weeks prior to experiment initiation. The hair of the dorsal back between the shoulders and hindquarters of three male and 3 female rabbits, 4 - 9 months of age at dosing, was closely shorn with fine electric clippers. A test site was selected and a 2 cm x 2 cm lint patch with 0.5 ml of sBA was applied to it. The patch and surrounding skin were covered by a single layer of gauze and held in place with an elastic adhesive bandage. The wrapping and patch were removed after 4 hours and the skin was not washed. The site was examined and scored for erythema and edema on a graded scale 0 - 4. Observations were made 30 minutes after the removal of the patch and at 24, 48, and 72 hours and 7 days following dosing. The mean scores for each rabbit at each observation time were calculated. There were no skin reactions following the application of sBA to rabbit skin for 4 hours. The test material is therefore not a skin irritant in rabbits.
Purity: 99.5%
Sex: Male and Female
Vehicle: None
Route of Administration: Dermal
Doses: 0.5 ml
Doses/Time: Single application
Post Dose Observation Period: After removal of patch: 0.5 hours; 24, 48, 72 hours and Day 7 after dosing.

Result	:	PII = 0
Conclusion	:	sBA caused no skin reaction and is not a skin irritant in rabbits.
Reliability	:	(1) valid without restriction 1 - Reliable without Restrictions. No circumstances occurred that would

have affected the quality or integrity of the data

10.01.2002 (73)

5.2.2 EYE IRRITATION

Species	:	rabbit
Concentration	:	
Dose	:	
Exposure time	:	
Comment	:	
Number of animals	:	5
Vehicle	:	
Result	:	irritating
Classification	:	irritating
Method	:	other: Experimental (Non-regulatory)
Year	:	1954
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Eye injury in rabbits records the degree of corneal narcosis from various volumes and concentrations of chemical, as detailed in Carpenter and Smyth (1946). Grade 1 indicates at most a very small area of narcosis resulting from 0.5 ml of undiluted chemical in the eye; Grade 5 indicates a so-called severe burn from 0.005 ml, and Grade 10 indicates a severe burn from 0.5 ml of a 1% solution in water or propylene glycol. Sex: Male Vehicle: None Route of Administration: Ocular application into the conjunctival sac of one eye Control: Untreated eye Dose: Single application of undiluted sBA Volume: 0.02 and 0.1 ml Post Dose Observation Period: 24 Hours
Result	:	Irritating (score 4/10); Severe injury from 0.1 ml, minor from 0.02 ml; Grade 4 eye injury.
Source	:	EXXON CHEMICAL, Limited Fareham, Hampshire EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Conclusion	:	sBA caused moderate damage and/or corneal opacity in rabbits.
Reliability	:	(2) valid with restrictions 2 - Reliable with restrictions: data are from a collection of data.

10.01.2002 (17) (82)

Species	:	rabbit
Concentration	:	
Dose	:	
Exposure time	:	
Comment	:	
Number of animals	:	6
Vehicle	:	
Result	:	corrosive
Classification	:	
Method	:	OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
Year	:	1986
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	New Zealand White rabbits, 3 - 6 months of age, were acclimated to the laboratory conditions for at least 2 weeks prior to experiment initiation. Three male and 3 female rabbits were 4 - 9 months of age at dosing. The day before testing, the eyes were carefully examined for any damage and

any animals showing damage were replaced. A single dose of 0.1 ml of sBA was placed into the lower conjunctival sac of one eye and the lids held together for a few seconds to prevent loss of material. The eyes were not washed. The reactions of the animal were observed and the initial pain responses graded on a 1 - 6 scale, no pain to very sever initial pain. Visual assessments were made 1, 5-7, 24, 28, and 72 hours and 7 Days postdosing. Irritancy was scored for the cornea, iris, and conjunctiva using standard scores. Any corneal damage visualization was aided by instillation of one drop of 2% fluorescein solution. The degree of irritation was classified using a scheme based on the OECD Data Interpretation Guide (1984). The instillation of undiluted sBA resulted in moderate initial pain. The conjunctival redness, chemosis and discharge, corneal opacity and damage to the iris were assessed and mean scores calculated. All rabbits had moderate conjunctival inflammation with some discharge within 1 hour of dosing. The swelling and discharge largely cleared by four hours but the redness persisted in 3 rabbits for 7 days. These 3 animals, and another, had impaired iritic response and/or slight corneal opacity between 24 and 72 hours postdosing. The effect had cleared by 7 days in 3 rabbits. The severely affected rabbit had a completely opaque cornea and no iritic response. It was humanely terminated since recovery was deemed not possible. The remaining rabbits were retained and by day 14 all ocular effects had cleared. In view of the responses, sBA is classified as corrosive to rabbit eyes (OECD, 1984).
Study Type: Ocular Irritation (Draize type)
Purity: 99.5%
Sex: Male and Female
Vehicle: None
Route of Administration: Ocular application into the conjunctival sac of one eye
Control: Untreated Eye
Dose: Single application of neat material
Volume: 0.1 ml
Post Dose Observation Period: 1, 5-7, 24, 28, and 72 hours and 7 Days postdosing

Result : Corrosive

Conclusion : sBA caused moderate conjunctival inflammation in all six rabbits with slight transitory iritic damage and/or corneal opacity in three rabbits. One rabbit developed intense, extensive corneal opacity and complete loss of iritic response. The test material was there for corrosive to the rabbit eye. On administration of sBA, there was a moderate initial pain response.

Reliability : (1) valid without restriction
1 - Reliable without Restrictions. No circumstances occurred that would have affected the quality or integrity of the data.

10.01.2002 (73)

5.3 SENSITIZATION

Type : Freund's complete adjuvant test
Species : guinea pig
Number of animals : 20
Vehicle : other: Corn oil
Result : not sensitizing
Classification : not sensitizing
Method : other: Magnusson and Kligman; 1969
Year : 1986
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Remark : Guinea pigs in the weight range of 300-370 grams were purchased from a commercial supplier and acclimated to the laboratory for at least 2 weeks.

The skin sensitization potential of sBA was assessed using the guinea pig maximization test of Magnusson and Kligman. The test was accomplished in 2 stages: rangefinding and definitive test.

Rangefinding:
The purpose of the rangefinding studies was to determine the concentrations of test material to be used for intradermal induction, topical induction and topical challenge. Two males and two female guinea pigs were closely shorn in the shoulder region using electric clippers followed by an electric razor and 0.1 ml of several dilutions (0.05, 0.1, 0.5 and 1.0% [m/v] in corn oil) of sBA injected intradermally each side of the midline. The animals were observed over the next few days to determine the maximum concentration that could be tolerated without causing untoward toxicity. Three further groups of two males and two females had their flanks closely shorn and 0.3 ml of several dilutions (25%, 50%, and 75% [m/v] in corn oil) of sBA were applied to a 4 cm x 4 cm Whatman Number 3 filter paper patches. The patches were placed on the flanks and held in place with a "Sleek" adhesive tape patch, then covered with a "Poroplast" elastic adhesive bandage for 24 hours. The bandages were removed and the animals were examined for signs of irritation and scored using a 4-point scale (0, 1, 2, and 3). The concentration used for topical induction was the one that scored 1 for irritation and the concentration for challenge was the one that was 0, a non-irritant.

Definitive:
This test was conducted using a group of ten male and ten female guinea pigs together with a control group of five males and five females. The test consisted of two stages: a) induction by intradermal injection and topical application, and, 2) topical challenge. The following concentrations were selected for the definitive study: Intradermal induction, 0.1% (m/v) in corn oil; Topical induction (one week following intradermal challenge), 50% (m/v) in corn oil and 25% (m/v) in corn oil. Topical challenge was carried out two weeks following the topical induction by applying 0.1 ml of the diluted sBA to a semi-occluded challenge patch and removing it 24 hours later. The erythema resulting from the topical challenge was scored on a 4-point scale (0, 1, 2, and 3) immediately on removal of the challenge patches and 24 and 48 hours latter. None of the twenty test animals showed any positive response at either 24 or 48 hours after the removal of the challenge patches. It was concluded that sBA was not a dermal sensitizer in guinea pigs.
Purity: 99.5%

Sex: Male and Female

Route of Administration: Intradermal and topical induction; topical challenge

Doses:
Intradermal Induction:
Test Doses:
2 injections (0.1 ml) of Freund's Complete Adjuvant (FCA)
2 injections (0.1 ml) of sBA in corn oil
2 injections (0.1 ml) of sBA in 50:50 FCA:corn oil
Control Doses:
2 injections (0.1 ml) of Freund's Complete Adjuvant (FCA)
2 injections (0.1 ml) of corn oil
2 injections (0.1 ml) of 50:50 FCA:corn oil
Topical Induction:
Application of 0.3 ml 50% sBA (m/v) in corn oil and, 25% sBA (m/v) in corn oil covered for 48 hours.
Topical Challenge:
Application 0.1 ml of diluted sBA to a semi-occluded challenge patch and

removing it 24 hours later.

Post Dose Observation Period: Immediately, 24 and 48 hours following challenge

Result : sBA is not a dermal sensitizer in guinea pigs.
Conclusion : In the guinea pig maximization test of Magnusson and Kligman, sBA did not induce positive responses in any of the 20 test animals at 24 or 48 hours after removal of the challenge patches. sBA is therefore not a dermal sensitizer in guinea pigs.
Reliability : (1) valid without restriction
1 - Reliable without Restrictions. No circumstances occurred that would have affected the quality or integrity of the data.

11.01.2002 (73)

Type : Guinea pig maximization test
Species : guinea pig
Number of animals : 20
Vehicle : other: Paraffin oil
Result : not sensitizing
Classification : not sensitizing
Method : other: OECD Guide-line 406 and EC92/69/EEC, B6
Year : 1992
GLP : yes
Test substance : other TS

Remark : Age: ~ 3 months

Sex: Male and Female

Weight (initial): Males 335 ± 17 g; Females 332 ± 19 g

Doses:
Intradermal Induction:
Test Doses:
Injections: sBA in paraffin oil (5% w/w)
sBA in FCA (Freund's Complete Adjuvant)
Control Doses:
Injections: Paraffin oil
Freund's Complete Adjuvant (FCA)
Topical Induction:
Application: sBA (undiluted) covered for 48 hours
Topical Challenge:
Application: sBA (undiluted) covered for 24 hours

Post Dose Observation Period: Skin reactions were evaluated at approximately 24 and 48 hours.
Clinical Signs: None

Rechallenge: None

Thirty guinea pigs were allocated to two groups: a control group 1 (five males and five females) and a treated group 2 (ten males and ten females). Day 1: Intradermal injections of Freund's complete adjuvant mixed with the test substance (treated group) or the vehicle (control group) were performed in the dorsal region between the shoulders. Day 7: The same dorsal region between the shoulders received a topical application of sodium lauryl sulfate in Vaseline (10% w/w) in order to induce local irritation.
Day 8: The test site was treated by topical application of the test substance (treated group) or the vehicle (control group) and was covered by an occlusive dressing for 48 hours.
Day 22: After a rest period of 12 days, all animals of the treated and control

groups were challenged by a topical application of the test substance to the right flank. The left flank served as control and received the vehicle only. Test substance and vehicle were maintained under an occlusive dressing for 24 hours. Skin reactions were evaluated approximately 24 and 48 hours later.

At the end of the study, animals were killed without examination of internal organs. No skin samples were taken from the challenge application sites.

The sensitivity of the guinea pigs was checked with a positive sensitizer: 2,4-dinitro chlorobenzene (DNCB). During the induction period, the test substance was applied at 0.1 % (w/w) (day 1) and 1 % (w/w) (day 8). For the challenge application, the DNCB was applied to the right flank at a concentration of 0.5% (w/w).

Result : sBA is not a dermal sensitizer in guinea pigs. The sensitivity of the guinea pigs was satisfactory since 50% of the animals showed a positive reaction with positive control sensitizer, DNCB. Scores in control and treated groups after challenge with sBA were 0 at both 24 and 48 hours.
Source : Centre d'Elevage Lebeau, Gambais, France
Test substance : sec-Butanol (sBA) 99.87%; ATOFINA Chemicals, Inc,
Conclusion : In the guinea pig maximization test of Magnusson and Kligman, sBA is not a dermal sensitizer.
Reliability : (1) valid without restriction
1 - Reliable without Restrictions.

11.01.2002 (32)

5.4 REPEATED DOSE TOXICITY

Type :
Species : rat
Sex : male
Strain : Sprague-Dawley
Route of admin. : inhalation
Exposure period : 3-5 days
Frequency of treatm. : 6 hours/day
Post exposure period :
Doses : 2000 ppm (3 Days) and 500 ppm (5 Days)
Control group :
Method : other: Experimental -- Study of changes in cytochrome P-450 enzyme system of rat liver, kidney and lung
Year : 1985
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Remark : Purity: > or = 99%
Number/Sex/Dose: 5
Vehicle: None
Result : sBA caused increases in cytochrome P-450 concentrations in the kidneys (47% rise; 500 ppm for 5 days) and liver (33% rise; 2000 ppm for 3 days). Slight decreases in lung cytochrome P-450 were observed.
Conclusion : sBA (probably through its metabolite methyl-ethyl-ketone) was a potent inducer of P-450 in the kidney and liver.
Reliability : (2) valid with restrictions
2- Reliable study with restrictions. Study well documented, meets generally accepted scientific principles, acceptable for assessment.

11.01.2002 (2)

Type :
Species : rat
Sex : male/female

Strain	:	Fischer 344
Route of admin.	:	inhalation
Exposure period	:	90 days
Frequency of treatm.	:	6 hours/day; 5 days/week
Post exposure period	:	
Doses	:	0, 1250, 2500, or 5000 ppm - Vapor
Control group	:	yes
NOAEL	:	= 2500 ppm
LOAEL	:	= 5000 ppm
Method	:	other: Comparable to OECD Guideline 413; 90-Day Subchronic Toxicity
Year	:	1981
GLP	:	yes
Test substance	:	other TS
Remark	:	An extensive pathologic investigation was conducted and no lesions were found that could be attributed to MEK exposure. There was no indication that repeated exposure to relatively high levels of MEK had any effect on reproductive tissues. The examined tissues included testes, epididymides, seminal vesicles, vagina, cervix, uterus, oviducts, and ovaries. Methyl ethyl ketone is metabolically interchangeable with 2-butanol. Approximately 97% of a 2-butanol dose is oxidized to methyl ethyl ketone. Purity: > 99.5% Number/Sex/Dose: 15 (10/sex - principals - for routine pathology and 5/sex - dedicated - for special neuropathology) Vehicle: None
Result	:	The 90-day exposures had no adverse effect on the clinical health or growth of male or female rats except for a depression of mean body weight in the 5000-ppm exposure group. No animals died during the study. No signs of nasal irritation were observed during the study. There were no treatment-related effects in food consumption or ophthalmologic studies in any of the rats exposed to MEK vapors. The 5000-ppm animals had a slight but significant increase in liver weight, liver weight/body weight ratio and liver weight/brain weight ratio at the time of necropsy. Serum glutamic-pyruvic transaminase (SGPT) activity in the 2500-ppm female rats was elevated while the 5000-ppm female rats exhibited significantly decreased SGPT activity. In addition, alkaline phosphatase, potassium, and glucose values for the 5000-ppm female rats were increased. Special neuropathological and routine pathological studies did not reveal any lesions that could be attributed to MEK exposure.
Source	:	EXXON CHEMICAL, Limited Fareham, Hampshire EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Test substance	:	Methyl Ethyl Ketone (MEK)
Conclusion	:	MEK has a low order of toxicity based on the 90-day repeated-dose exposures. The NOAEL is 2500 ppm.
Reliability	:	(1) valid without restriction 1 - Reliable study with restrictions. Study well documented, meets generally accepted scientific principles, acceptable for assessment.

14.01.2002 (19) (89)

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Ames test
System of testing	:	Bacterial
Test concentration	:	0.01, 0.1, 0.5, 1.0, and 5.0 mg/ml
Cycotoxic concentr.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	OECD Guide-line 471
Year	:	1985

GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Purity: 99.5% Strain: S. typhimurium / TA98, TA100, TA1535, TA1537, TA1538 Species/Cell Type: Rat Liver (S9 fraction) Vehicle: DMSO sBA did not induce reverse gene mutation in bacteria.
Source	:	EXXON CHEMICAL, Limited Fareham, Hampshire EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Test condition	:	Control plates were set up with solvent alone and with an appropriate known positive control compound. All tests were carried out in triplicate. Two replicate assays were carried on different days in order to confirm the reproducibility of the results. The S9 fractions were prepared from Aroclor-induced rats. Initially, a range of test concentrations of test material was tested and a second experiment was then performed based on the results taking into account the effect on cell viability and any possible positive increases in mitotic gene conversion. Control plates were set up with solvent alone and with the positive control compounds 4-nitroquinoline-N-oxide and cyclophosphamide.
Conclusion	:	Not Mutagenic
Reliability	:	(1) valid without restriction 1- Reliable without restriction

11.01.2002 (15)

Type	:	Ames test
System of testing	:	Bacterial
Test concentration	:	0.01, 0.1, 0.5, 1.0, and 5.0 mg/ml
Cycotoxic concentr.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	OECD Guide-line 472
Year	:	1985
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Purity: 99.5% Strain: E. coli WP2 uvr A Species/Cell Type: Rat Liver (S9 fraction) Vehicle: DMSO sBA did not induce reverse gene mutation in bacteria.
Source	:	EXXON CHEMICAL, Limited Fareham, Hampshire EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Test condition	:	Control plates were set up with solvent alone and with an appropriate known positive control compound. All tests were carried out in triplicate. Two replicate assays were carried on different days in order to confirm the reproducibility of the results. The S9 fractions were prepared from Aroclor-induced rats. Initially, a range of test concentrations of test material was tested and a second experiment was then performed based on the results taking into account the effect on cell viability and any possible positive increases in mitotic gene conversion. Control plates were set up with solvent alone and with the positive control compounds 4-nitroquinoline-N-oxide and cyclophosphamide.
Conclusion	:	Not Mutagenic
Reliability	:	(1) valid without restriction 1- Reliable without restriction.

14.01.2002 (15)

Type	:	other: Yeast mitotic gene conversion
System of testing	:	Saccharomyces cerevisiae
Test concentration	:	Maximum conc. 5 mg/ml
Cycotoxic concentr.	:	

Metabolic activation	:	with and without
Result	:	negative
Method	:	OECD Guide-line 481
Year	:	1988
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Purity: 99.5% Strain: Saccharomyces cerevisiae Species/Cell Type: Rat Liver (S9 fraction) Vehicle: DMSO sBA did not induce mitotic gene conversion in yeast.
Source	:	EXXON CHEMICAL, Limited Fareham, Hampshire EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Test condition	:	Yeast cells were grown in log phase, washed and re-suspended in 2/5 strength YEPD broth at a concentration of 10 X 106cells/ml. The suspension was then divided into 1.9 ml amounts in 30-ml universal containers and 0.1 ml of the test compound solution was added (-S9). For the experiments with metabolic activation (+S9), 0.1 ml of the compound was added to 1.6 ml of yeast suspension, together with 0.3 ml of S9 mix. The cultures were incubated with shaking, with shaking, at 30°C for 18 hours. Aliquots were then plated onto the appropriate culture media for the selection of mitotic gene convertants and cells surviving the treatment.
Conclusion	:	Not mutagenic
Reliability	:	(1) valid without restriction 1- Reliable without restriction

14.01.2002 (14)

Type	:	other: chromosome abberration assay
System of testing	:	Chinese hamster ovary cells
Test concentration	:	maximum conc. 5000 ug/ml
Cycotoxic concentr.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	OECD Guide-line 473
Year	:	1988
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Purity: 99.5% Species/Cell Type: Chinese Hamster Ovary Cells Vehicle: DMSO sBA did not induce chromosome damage in CHO mammalian cells.
Result	:	Negative - No increase in chromosomal aberrations
Source	:	EXXON CHEMICAL, Limited Fareham, Hampshire EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Test condition	:	Two separate cytotoxicity assays were performed: (i) Monolayer CHO cultures were prepared in multi-well tissue culture trays. The cultures were incubated at 37°C for 24 hours to commence active growth before treatment with the test material. Assays were performed both in the presence and in the absence of S9 mix using either a 5-hour exposure (+S9) or a 24-hour exposure (-S9). Twenty-four hours after initial treatment, cultures were stained with Giemsa and the growth inhibition was noted. (ii) CHO cultures were prepared in 25 cm2 flasks, and after 24 hours the cells were exposed to sBA both in the presence and in the absence of S9 mix. The number of cell in each flask was counted 24 hours later. The compound concentrations selected for the chromosome assays were 1, 0.5, and 0.25 times the GI50 level. CHO Chromosome Assay: Cultured CHO cells were grown in 80-cm2 flasks for 24 hours before treatment. Treatment periods were 5hours in the presence of S9 mix and 24 hours in the absence of S9 mix. Positive control

cultures were run in parallel [ethyl methanesulphonate (-S9) and cyclophosphamide (+S9). Colcemid was added to all cultures 22 hours after treatment. After a further 2 hours, the cells were trypsinized, resuspended in hypotonic solution and then fixative, before spotting onto slides. Cell preparations were then stained with Giemsa. The slides were randomly coded and 100 cells from each culture were analyzed microscopically. Mitotic index estimations were also made.

Conclusion : Not Mutagenic
Reliability : (1) valid without restriction
1- Reliable without restriction

14.01.2002 (14)

Type : Ames test
System of testing : Bacterial
Test concentration : 100-500-1000-5000-10000 ug/plate
Cycotoxic concentr. :
Metabolic activation : with and without
Result : negative
Method : OECD Guide-line 471
Year : 1988
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Remark : sBA did not induce reverse gene mutation in bacteria.
Strain: Salmonella typhimurium / TA98, TA100, TA1535, TA1537, TA1538
Species/Cell Type: Rat Liver (S9 fraction)
Vehicle: DMSO
Source : EXXON CHEMICAL, Limited Fareham, Hampshire
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Test condition : Control plates were set up with solvent alone and with an appropriate known positive control compound. All tests were carried out in triplicate. Two replicate assays were carried out on different days in order to confirm the reproducibility of the results. The S9 fractions were prepared from Aroclor -induced rats. Initially, a range of test concentrations of test material was tested and a second experiment was then performed based on the results taking into account the effect on cell viability and any possible positive increases in mitotic gene conversion. Control plates were set up with solvent alone and with the positive control compounds 4-nitroquinoline-N-oxide and cyclophosphamide.
Conclusion : Not Mutagenic
Reliability : (1) valid without restriction
1- Reliable without restriction

11.01.2002 (31)

5.6 GENETIC TOXICITY 'IN VIVO'

Type : other: In Vivo Mammalian Bone Marrow Erythrocyte Micronucleus Assay Intraperitoneal Dosing Method
Species : mouse
Sex : male/female
Strain : CD-1
Route of admin. : other: Intraperitoneal injection
Exposure period : 12, 24 and 48 hours
Doses : 1.96 ml/kg Single injection
Result :
Method : other: OECD 474 equivalent
Year : 1988
GLP : no data
Test substance : other TS

Remark	:	Not mutagenic Purity: 99.9% Number: 5/sex/dose Dose/Time: 1.96 ml/kg Single injection (dose equal to the MEK LD20 reported as ml test article / kg body weight when administered in a total volume of 10 ml test article-vehicle mixture / kg body weight). Vehicle: Corn Oil (10 ml/kg) Positive Control: 0.25 mg/kg Triethylene melamine (TEM) The test substance and the vehicle were administered as a single dose by intraperitoneal injection. The vehicle was dosed at a volume equal to the test substance volume. The positive control was administered as a single dose at a volume equal to the test substance volume. Animals from the appropriate groups were sacrificed at approximately 12, 24 and 48 hours. Animals dosed with triethylene melamine were sacrificed at 24 hours only. Immediately following sacrifice, the femur was exposed and the bone marrow was aspirated into a syringe containing fetal calf serum. The cells were washed, centrifuged, and resuspended. Slide smears of the bone marrow were made for each animal and stained with May-Gruenwald-Giemsa stain. Coded slides were then evaluated for presence of micronuclei (1000 polychromatic erythrocytes/animal were evaluated). A 1-way analysis of variance and Duncan's multiple range test (p = 0.05) were used to assess the statistical significance of any observed effects.
Result	:	None of the dose groups were statistically different from the vehicle control. The positive control (0.25 mg/kg TEM) induced a statistically significant increase in the mean number of micronucleated polychromatic erythrocytes (p = 0.01) which indicates that the positive control was clastogenic and the test system responded in an appropriate manner. Vehicle carrier control values for the mean percent of polychromatic erythrocytes and for the mean percent of micronucleated polychromatic erythrocytes responded in an appropriate manner.
Test substance	:	Methyl Ethyl Ketone (MEK) CAS No. 78-93-3
Conclusion	:	MEK did not induce a statistically significant increase in the mean number of micronucleated polychromatic erythrocytes in the bone marrow of CD-1 mice. Therefore, it is not considered mutagenic under the conditions of this assay.
Reliability	:	(1) valid without restriction 1 - Reliable without Restrictions. No circumstances occurred that would have affected the quality or integrity of the data.

29.01.2002 (70)

Type	:	other: Rat Bone Marrow
Species	:	rat
Sex	:	no data
Strain	:	no data
Route of admin.	:	other: intragastric
Exposure period	:	
Doses	:	
Result	:	
Method	:	other: Micronucleus Aberration
Year	:	1988
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Single intragastric administration of monohydric alcohols at equitoxic doses (1/5 LD50) affected the chromosomal appearance of bone marrow. System of Testing: Rat Bone Marrow Metabolic Activation: unknown Species/Cell Type: Rat Concentrations Tested: 1/5 of the LD50 by intragastric route Vehicle: unknown
Result	:	Increased numbers of polyploid cells, cells with chromosome gaps, and cells with chromosomal aberrations.

Conclusion : unknown
Reliability : (4) not assignable
4 - Incomplete translation from Russian and insufficient for assessment

11.01.2002 (5)

5.7 CARCINOGENICITY

Remark : No studies of 2-butanol for carcinogenic activity have been reported; however, based on results of mutagenicity assays it is expected to have a low potential for carcinogenicity.
Source : EXXON CHEMICAL, Limited Fareham, Hampshire
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

21.10.1992

5.8.1 TOXICITY TO FERTILITY

Type : other: two generation study with teratology screen
Species : rat
Sex : male/female
Strain : Wistar
Route of admin. : drinking water
Exposure period :
Frequency of treatm. : Daily - ad libitum
Premating exposure period
Male : 8 weeks
Female : 8 weeks
Duration of test : 2 Generations
No. of generation studies :
Doses : F0 Generation: 0, 0.3, 1.0, or 3.0% solutions; F1 Generation: 0, 0.3, 1.0, or 2.0%
Control group : yes
NOAEL F1 offspring : = 1 %
other: NOAEL Maternal : = 1 %
Method : other: Comparable to an OECD 416 guideline study.
Year : 1975
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : Purity: > or = 99%

Number/Sex/Dose: 30

Doses/Concentration:
F0 Generation: 0, 0.3, 1.0, or 3.0% solutions (0, 538, 1644, and 5089 mg/kg-day for males and 0, 594, 1771, and 4571 mg/kg-day for females)
F1 Generation: 0, 0.3, 1.0, or 2.0% (2.0% calculated to be equivalent to 3384 mg/kg-day for males and 3122 mg/kg-day for females)

Vehicle: Drinking Water
sec-Butanol was initially administered to the F0 generation at concentrations of 0, 0.3, 1.0, and 3.0% in the drinking water. Due to toxicity, the high level was reduced to 2.0% during the second-generation study (F1). The F1 generation animals (30/sex/group) were reared to maturity (up to week 12), mated to produce a F2 generation, then sacrificed for organ weights, and gross and microscopic pathological evaluations

(10/sex/group). Hematological, biochemical, and urinary examinations were conducted terminally on the F1 rats. A series of mild changes in the kidney (non-reactive tubular degeneration, tubular casts, foci of tubular regeneration, microcysts) were observed animals treated at 2.0% sBA. The authors concluded that these findings were not a result of direct toxicity and did not have clear pathologic significance. Rather they were non-specific effects due to increased renal work load, possibly from increased urine volume and pressure at the high dose of sBA (Cox et al, 1975). No other findings of note were seen. The no-effect level for the study was 1.0% (estimated to be 1500 mg/kg/day by the authors and 1771 mg/kg/day by EPA/IRIS).

Result : Maternal NOEL: 1% (~1500 mg/kg/day)
Maternal NOAEL: 1771 mg/kg/day
Pup NOEL: 1% (~1500 mg/kg/day)
Pup NOAEL: 1771 mg/kg/day

Source : EXXON CHEMICAL, Limited Fareham, Hampshire
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Conclusion : sBA is not a reproductive hazard.

Reliability : (2) valid with restrictions
2 - Reliable study with restrictions. No circumstances occurred that would have affected the quality or integrity of the data. Comparable to a guideline study and test procedures were in accordance with generally accepted scientific standards and described in sufficient detail.

11.01.2002 (22) (40)

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species : rat
Sex : female
Strain : Sprague-Dawley
Route of admin. : inhalation
Exposure period : Gestation Days 1-19
Frequency of treatm. : 7 hr/day
Duration of test : 20 days
Doses : 3500, 5000, 7000 ppm
Control group : yes
NOAEL maternal tox. : = 3500 ppm
NOAEL teratogen. : > 7000 - ppm
Method : other: Comparable to an OECD 414 guideline study
Year : 1989
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Method : For the maternal data, multivariate analysis (with baseline as covariant) was used for weight comparisons across groups. The group differences in food and water intake were analyzed by multivariate analysis of variance. A Kruskal-Wallis test was used for group comparisons of corpora lutea per animal. For the fetal data, analysis of covariance was used to compare fetal weights across groups and sex. Group comparisons of the variables including litter size, percentage alive/litter, percentage normal/litter, and percentage females/litter were made using Kruskal-Wallis test. For the variables including skeletal malformations, skeletal variations, visceral malformations, visceral variations, external malformations, and non-normal fetuses, the number of litters with one or more of the variables of interest was compared between groups using Fisher's exact test. The results of the test were adjusted for multiple comparisons, when appropriate, using the Bonferroni technique. A probability of $p = < 0.05$ was required for significance.

Remark : Groups of 15-16 rats were exposed by inhalation to 0, 3,500, 5,000 or 7,000 ppm sBA, 7 hours/day on days 1-19 of gestation; the dams were

sacrificed on day 20. At 7,000 ppm, narcosis was observed in all animals. At 5000 ppm, the dams were partially narcotized with locomotion activity impaired. Maternal weight gain and food consumption were significantly reduced in all dose groups. No data collected on maternal organ weights, or gross or microscopic lesions. The number of live fetuses was significantly reduced and resorptions were increased in the high exposure group only. Fetal body weights were significantly reduced in the mid- and high dose groups. There was no evidence of teratogenic effects in this study, and there was also no evidence of selective developmental toxicity. The no-effect levels were < 3,500 ppm for maternal toxicity and 3,500 ppm for developmental toxicity.
Purity: > or = 99%
Number/Sex/Dose: 15-16 Mated Females
Vehicle: None

Result : Maternal NOEL: < 3500 ppm
Maternal NOAEL: 3500 ppm
Pup NOEL: 3500 ppm
Pup NOAEL: > 7000 ppm

Source : EXXON CHEMICAL, Limited Fareham, Hampshire
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Conclusion : sBA is not a teratogen. There was no evidence of teratogenic events nor was there evidence of selective developmental toxicity.

Reliability : (2) valid with restrictions
2- Reliable study with restrictions. Study well documented, meets generally accepted scientific principles, acceptable for assessment.

14.01.2002 (69)

Species : rat
Sex : female
Strain : Wistar
Route of admin. : drinking water
Exposure period : 8 Weeks premating (Males and Females) and during gestation (Females)
Frequency of treatm. : Daily - ad libitum
Duration of test : 20 days
Doses : 0, 0.3, 1.0, or 2.0% solutions
Control group : yes
Method : other: Comparable to an OECD 421 guideline study.
Year : 1975
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : Purity: > or = 99%
Doses/Concentration: F0 Generation - second breeding.
0, 0.3, 1.0, or 2.0% solutions (0, 538, 1644, and 3384 mg/kg-day for males and 0, 594, 1771, and 3122 mg/kg-day for females)
Vehicle: Drinking Water
Number/Sex/Dose: 30
TERATOLOGY SCREEN RESULT: The F0 rats were mated to obtain a second series of pregnant dams destined to provide teratologic evaluation of the treatments. Pregnancy rates and survival of these females were unaffected. All findings sBA at both 0.3 and 1.0% in the drinking water were negative with respect to signs of toxicity in terms of both growth and reproductive efficiency The body weights of the dams were not depressed. Examination of the uterine contents on the 20th day of gestation revealed that sBA was somewhat fetotoxic at the 2.0% dosage level, as shown by the decreased pup weights (3.74 g vs. 4.14 g in controls). However, that this is a minimal response is shown by the fact that none of the other parameters in the reproductive toxicity phase of this study (nidation, early or late fetal deaths) were affected. The 2.0% group showed apparent increases in missing sternebrae, wavy ribs, and incomplete vertebra ossification when compared with both the 0.3 and 1.0% groups. However, because the incidences for these findings in the control group were

comparable, these effects could not be determined to be compound-related. The skeletal abnormalities seen in the sBA groups were consistent in type and frequency with the spontaneous incidence observed in this rat colony. There were no significant soft tissue findings in the 2% treated group.

Result : Maternal NOEL: 1% (1771 mg/kg/day)
Maternal NOAEL: 1% (1771 mg/kg/day)
Pup NOEL: 1% (1771 mg/kg/day)

Conclusion : Not a teratogen.

Reliability : (2) valid with restrictions
2 - Reliable study with restrictions. No circumstances occurred that would have affected the quality or integrity of the data. Comparable to a guideline study and test procedures were in accordance with generally accepted scientific standards and described in sufficient detail.

11.01.2002 (22) (40)

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

Remark : Excessive exposure by inhalation may result in headache, dizziness, drowsiness and narcosis. No adverse systemic effects due to exposure to 2-butanol have been reported in man.

Source : EXXON CHEMICAL, Limited Fareham, Hampshire
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

22.10.1992 (35)

5.11 ADDITIONAL REMARKS

Type : other: Respiratory Irritation

Remark : Respiratory rates of CF-1 mice (mean weight 25 g.) were determined prior to exposure. SBA was evaporated, diluted with room air and fed into a 3.3 liter chamber at an airflow rate of 18.3 to 26.9 l/min. Each animal was placed in a body plethysmograph attached to the exposure chamber so that the head of the animal protruded into the chamber. The respiratory rate and the relative tidal volume were obtained by attaching a pressure transducer to each plethysmograph. The results were expressed as percentage of pre-exposure values, obtained from a 10-minute control period. The exposure was 30 minutes, followed by a 20-minute recovery period during which the respiratory pattern and respiratory rate were monitored continuously. Respiration rates and tidal volumes were compared between normal and cannulated mice to determine the on-set and extent of respiratory irritation. In the cannulated mice, the onset of the decrease in respiration was slower than that of the normal mice indicating that sBA was acting as a respiratory irritant.
Species/Strain: Mouse / CF-1
Sex: Male
Number/Sex/Dose: 10
Vehicle: None
Route of Administration: Inhalation

Doses: 2800, 5600, 10100 or 15300 ppm normal mice;
10500 or 14000 ppm cannulated mice
Time of Exposure: 30 minute
Post Dose Observation Period: 20 minute
Method: Alarie Test
GLP: Unknown
Year: 1994

Result : 640 ppm RD0 Threshold Concentration at 2 minutes;
11800 ppm RD50 at 10 minutes

Test substance : sec-Butanol (sBA)

Conclusion : sBA caused a concentration-dependent decrease in respiratory tidal volume in normal and cannulated mice and acts as a respiratory irritant.

Reliability : (1) valid without restriction
1 - Reliable without Restrictions. No circumstances occurred that would have affected the quality or integrity of the data.

11.01.2002 (48)

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

(1) 1992-1993 Threshold Limit values and Biological Exposure Indices ACGIH

(2) Aarstad K., Zahlsen, K., and Nilsen, O. G. (1985). Inhalation of butanols: changes in the cytochrome p-450 enzyme system. Arch Toxycol (Suppl) 8:418-421.

(3) ACGIH list 1993-1994

(4) Applegate, V.C. et al. 1957. Toxicity of 4,346 chemicals to larval lampreys and fishes. Special Scientific Report--Fisheries No. 207. US Dept. of the Interior, US Fish and Wildlife Service, Washington, DC, USA.

(5) Barilyak, I. R. and Kozachuk, SYu. (1988). Investigation of the cytogenetic effect of a number of monohydric alcohols on rat bone marrow cells. Cytology and Genetics (Tsitologiaya I Genetika), 22(2):49-52.

(6) Bridie, A.L., C.J.M. Wolff, and M. Winter. 1979. BOD and COD of Some Petrochemicals. Water Research. 13:627-630.

(7) Bridie, A.L., C.J.M. Wolff, and M. Winter. 1979. The Acute Toxicity of Some Petrochemicals to Goldfish. Water Research. 13:623-626.

(8) Bringmann, G. and Kuhn, R. 1976. Vergleichende Befunde der Schadwirkung wassergefahrdender Stoffe gegen Bakterien (Pseudomonas putida) und Blaualgen (Microcystis aeruginosa). Gwf-Wasser/Abwasser, Vol. 117.

(9) Bringmann, G. and Kuhn, R. 1977. Results of the damaging effect of water pollutants on Daphnia magna. Z. Wasser Abwasser Forsch., 10(5):161-166.

(10) Bringmann, G. and Kuhn, R. 1980. Bestimmung der biologischen Schadwirkung wassergefahrdender Stoffe gegen Protozoen. II. Bakterienfressende Ciliaten. Z. Wasser/Abwasser Forsch., 1:26-31.

(11) Bringmann, G. and Kuhn, R. 1980. Comparison of the toxicity thresholds of water pollutants to bacteria, algae and protozoa in the cell multiplication inhibition test. Water Research, 14:231-241.

(12) Bringmann, G. and R. Kuhn. 1980. Comparison of the toxicity thresholds of water pollutants to bacteria, algae and protozoa in the cell multiplication inhibition test. Water Research, 14:231-241.

(13) Bringmann, G. and R. Kuhn. 1980. Comparison of the Toxicity Thresholds of Water Pollutants to Bacteria, Algae, and Protozoa in the Cell Multiplication Inhibition Test. Water Research. 14:231-241.

(14) Brooks, T. M., Meyer, A., and Hutson, D. H. (1988). The genetic toxicology of some hydrocarbon and oxygenated solvents. Mutagenesis, 3(3):227-231.

(15) Brooks, T. M., Meyer, A., and Hutson, D. H. (1988). The genetic toxicology of some hydrocarbon and oxygenated solvents. Mutagenesis, 3(3):227-231.

(16) Bysshe, S.E. 1982. Biconcentration Factor in Aquatic Organisms. In: Handbook of Chemical Property Estimation Methods. Environmental Behavior of Organic Compounds. 5, 1-43. Lyman W.J., Reehl, W.F., and Rosenblatt, D.H. (eds). McGraw-Hill, New York, NY, USA.

(17) Carpenter, C.P., and Smith, H. F. Jr,. (1946). Chemical Burns of the Rabbit Cornea. Am. J. Ophth. 29:1363.

(18) Cash, G. and V. Nabholz.. 1999. ECOSAR Classes for Microsoft Windows, ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment Division. Washington, DC, USA.

(19) Cavender, F.L., Casey, H.W., Salem, H., Swenberg, J.A., and Gralla, E.J. (1983). A 90-day vapor inhalation toxicity study of methyl ethyl ketone. Fund. Appl. Toxicol. 3:264-270.

(20) Chemcial Hazard Assessment Division, Syracuse Research Corp. 1988. Syracuse, NY, USA.

(21) Chou, W.L. et.al. 1979. Bio. Eng. Symp. 8, 391-414.

(22) Cox, G.E., D.E. Bailey and K. Morgareidge. (1975). Toxicity studies in rats with 2-butanol including growth, reproduction and teratologic observations. LaB No. 2093. Food and Drug Research Laboratories, Inc., Waverly, NY.

(23) CRC Handbook of Chemistry and Physics. Lide, D. R., ed. 81st Edition, pp. 3-100. CRC Press LLC, Boca Raton, FL. 2000.

(24) de Zwart, D. and Slooff, W. 1987. Toxicity of Mixtures of Heavy Metals and Petrochemicals to Xenopus laevis. Bull. Environ. Contam. Toxicol., 38:345-351.

(25) Dietz FK, Rodrigues-Giaxola M, Traiger GJ, Stella VJ and Himmelstein KJ (1981). Pharmacokinetics of 2-Butanol and its metabolites in the rat. Journal of Pharmacokinetics and Biopharmaceutics 9(5), 553-576.

(26) Dilling, W. L. et. al. (1976). Organic Photochemistry. Simulated atmospheric photodecomposition rates of methylene chloride, 1,1,1-trichloroethane, trichloroethylene, tetrachloroethylene, and other compounds. Env. Sci. Technol. 10(4), 351-356.

(27) DiVincenzo GD, Kaplan CJ and Dedinas J (1976). Characterization of the metabolites of Methyl n-Butyl Ketone, Methyl iso-Butyl Ketone, and Methyl Ethyl Ketone in guinea pig serum and their clearance. Toxicology and Applied Pharmacology 36, 511-522.

(28) Dore et al. 1975. Trib. Cebedeau, 27:3-11.

(29) Dutch MAC list 1994

(30) Edney, E.O. and Corse, E.W. 1986. Hydroxyl radical rate constant intercomparison study. EPA/600/3-86/056, US EPA, Research Triangle Park, NC, US.

(31) ELF ATOCHEM, BUTANOL SECONDAIRE TEST DE AMES "essai de mutation reverse sur Salmonella typhirium" SANOFI RECHERCHE Report CEL357A/C, 1989.

(32) Elf Atochem, Centre International de Toxicologie. 1997. Skin sensitization in guinea pigs (Maximization method of Magnusson, B. and Kligman, A.M.). Report # 14861 TSG.

(33) Environmental Health Criteria 65, Butanols: Four Isomers. World Health Organization, 1987.

(34) Environmental Health Criteria 65, World Health Organization, 1987.

(35) Environmental Health Criteria 65. Butanols: Four Isomers. World Health Organization, 1987.

(36) Environmental Health Criteria 65: Butanols: four isomers: 1-butanol, 2-butanol, tert-butanol, isobutanol. 1987. IPCS International Programme on Chemical Safety, World Health Organization.

(37) EPIWIN. 1999. Estimation Program Interface for Windows, Version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

(38) Ethel Browning's Toxicity and Metabolism of Industrial Solvents. Snyder, R., ed. Second Edition. Volume 3 Alcohols and Esters. New York, NY: Elsevier, 1992.

(39) EXXON CHEMICAL, Limited Fareham, Hampshire

(40) Gallo, M.A., Oser, B.L., Cox, G.E., and Bailey, D.E. (1977). Studies on the long-term toxicity of 2-butanol. Toxicology and Applied Pharmacology, 41:135 (Abstract).

(41) Geiger D.L. et al. 1986. Acute Toxicities of Organic Chemicals to Fathead Minnows (Pimephales promelas), Vol. 3. Center for Lake Superior Environmental Studies. University of Wisconsin-Superior, WS, USA.

(42) Gerhold and Malaney. 1966. J. Water Pollution Control Fed., 38:562-579.

(43) Great Lakes Water Quality Board. 1983. Inventory of Chemical Substances Indentified in the Great Lakes Ecosystem. Report to the Great Lakes Water Quality Board, Windsor, Canada.

(44) Gudjonsdottir, S. and Burstrom, H. 1962. Physl. Plant, 15:498-504.

(45) Gudjonsdottir, S. and Burstrom, H. Physl. Plant, 15:498-504.

(46) Handbook of Environmental Data on Organic Chemicals, Second Edition. Karel Verschueren, ed., Van Nostrand Reinhold Company (1983), pp. 301-302.

(47) Hansch, C., Leo, A., Hoekman, D. 1995. Exploring QSAR - Hydrophobic, Electronic, and Steric Constants. American Chemical Society, Washington, DC, USA.

(48) Hansen, L.F., and Nielsen, G.D. (1994). Sensory irritation, pulmonary irritation and structure-activity relationships of alcohols. Toxicol., 88:81-99.

(49) Harris, J.C. 1982. Rate of Hydrolysis. In: Handbook of Chemical Property Estimation Methods. Environmental Behavior of Organic Compounds. 7, 1-48. Lyman W.J., Reehl, W.F., and Rosenblatt, D.H. (eds). McGraw-Hill, New York, NY, USA.

(50) Hawley's Condensed Chemical Dictionary. Lewis, R. J., Sr., ed. 13th ed. New York, NY: John Wiley & Sons, Inc. 1997.

(51) Hefter, G.T. 1984. Solub. Data Ser., 15:94-119.

(52) INRS, Valeurs limites d'exposition professionnelle aux agents chimiques en France, Cah. Notes Doc. 1993, 153, 557-574

(53) INRS, Valeurs limites d'exposition professionnelle aux substances dangereuses de l'ACGIH aux Etats-Unis et de la Commission MAK en Allemagne, Cah. Notes Doc. 1992, 147, 195-225

(54) Jones, H.R. 1971. Environmental control in the organic and petrochemical industries. Noyes Data Corporation.

(55) Juhnke, I. and Luedemann, D. 1978. Results of the investigation of 200 chemical compounds for acute fish toxicity with the golden orfe test. Z. Wasser. Abwasser Forsch., 11(5):161-164.

(56) Juttner, F. 1986. Chemosphere, 15: 985-992.

(57) Karel Verschueren. 1983. Handbook of Environmental Data on Organic Chemicals, 2nd Edition. Karel Verschueren (ed), pp. 301-302. Van Nostrand Reinhold Company, New York, NY, USA.

(58) Kuhn, R., M. Pattard, K-D. Pernak and A. Winter. 1989. Results of the Harmful Effects of Selected Water Pollutants (Anilines, Phenols, Aliphatic Compounds) to Daphnia magna. Water Research. 14:495-499.

(59) Lamb, C.B. and G.F. Jenkins. 1953. B.O.D. of Synthetic Organic Chemicals. Procedings of the 7th Industrial Waste Conference. pp. 326-339.

(60) Liira J, Riihimaki V and Pfaffli P (1988). Kinetics of methyl ethyl ketone in man: absorption, distribution and elimination in inhalation exposure. Int.Arch. Occup. Environ. Health 60, 195-200.

(61) Lucas, S.V. 1984. GC/MS Analysis of organics in drinking water concentrates and advanced treatment concentrates. Vol. 1. USEPA-600/1-84-020a (NTIS).

(62) Lyman, W.J. (1982). Adsorption Coefficient for Soils and Sediments. In: Handbook of Chemical Property Estimation Methods. Environmental Behavior of Organic Compounds. 4,1-33. Lyman W.J., Reehl, W.F., and Rosenblatt, D.H. (eds). McGraw-Hill, New York, NY, USA.

(63) Macht, D.I. and Meyer, J.D. 1933. Am. J. Botany, 20:145-149.

(64) Mackay, D. 1998. Level I Fugacity-Based Environmental Equilibrium Partitioning Model, Version 2.1 (16-bit). Environmental Modelling Centre, Trent University, Ontario, Canada.

(65) Mellon (Mellon Institute of Industrial Research). (1951). "Project Report Number 14-78". Union Carbide Corporation, Danbury, CT, USA.

(66) Miller, L.P. 1934. Contr. Boy. T., 6:279-296.

(67) Munch, J.C. (1972). Aliphatic alcohols and alkyl esters: narcotic and lethal potencies to tadpoles and to rabbits. Ind. Med. 41:31-33.

(68) Munch, J.C. and Schwartze, E.W. (1925). Narcotic and toxic potency of aliphatic alcohols upon rabbits. J Lab Clin Med, 10:985-996.

(69) Nelson, B. K., Brightwell, W. S., Khan, A., Burg, J. R., and Goad, P. T. (1989). Lack of selective developmental toxicity of three butanol isomers administered by inhalation to rats. Fundam Appl Toxicol, 12:469-479.

(70) O'Donoghue, J.L., Haworth, S.R., Curren, R.D., Kirby, P.E., Lawlor, T., Moran, E.J., Phillips, R.D., Putnam, D.L., Rogers-Back, A.M., Slesinski, R.S., and Thilagar, A. (1988). Mutagenicity studies on ketone solvents: methyl ethyl ketone, methyl isobutyl ketone, and isophorone. Mutation Research, 206:149-161.

(71) Pitter. 1976. Water Research, 10:231-235.

(72) Price, J. B. (1986). Toxicology of industrial chemicals (solvents): The acute oral and percutaneous toxicity, skin and eye irritancy and skin sensitizing potential of secondary butyl alcohol. Shell Research Report SBGR.86.108. Shell Research Limited, Sittingbourne Research Centre.

(73) Price, J. B. (1986). Toxicology of industrial chemicals (solvents): The acute oral and percutaneous toxicity, skin and eye irritancy and skin sensitizing potential of secondary butyl alcohol. Shell research Report SBGR.86.108. Shell Research Limited, Sittingbourne Research Centre.

(74) Safety Data Sheet (sec-butanol), June 1990, ELF ATOCHEM.

(75) Safety Data Sheet ELF ATOCHEM June 1990

(76) Safety Data Sheet ELF ATOCHEM June 1990¿

(77) Sasaki, S. 1978. pp 283-298 in Aquatic Pollutants: Transfer and biological effects. Hutzinger, O. et. al. (eds.) Pergamon Press.

(78) Sawhney, B.L. and Kozloski, R.P. 1984. J. Environ. Qual. 13:349-352.

(79) Schultz, W. and M. Tichy. 1993. Structure-Toxicity Relationships for Unsaturated Alcohols to Tetrahymena pyriformis: C5 and C6 Analogs and Primary Propargylic Alcohols. Environ. Contam. and Toxicology. 51:681-688.

(80) Shackelford, W.M. et al. 1983. Analyt. Chim. Acta, 146:15-27 (supplemental data).

(81) Shell International Petroleum, B.V.

(82) Smyth, H. F. Jr, Carpenter, C. P., Weil, C. S., and Pozzani, U. C. (1954). Range-finding toxicity data: List V. Arch Ind Hyg Occup Med, 10:61-68.

(83) Smyth, H. F. Jr., Carpenter, C. P., Weil, C. S., and Pozzani, U. C. (1954). Range-finding toxicity data: List V. Arch Ind Hyg Occup Med, 10:61-68.

(84) Snider, J.R. and Dawson, G.A. 1985. J. Geophys. Res., 90:3797-3805.

(85) Starrek, E. (1938). Dissertation, Wirzburg.

(86) Thomas, R.G. 1982. Volatilization from Water. In: Handbook of Chemical Property Estimation Methods. Environmental Behavior of Organic Compounds. 15, 1-34. Lyman W.J., Reehl, W.F., and Rosenblatt, D.H. (eds). McGraw-Hill, New York, NY, USA.

(87) Thomas, R.G. 1982. Volatilzation from Soil. In: Handbook of Chemical Property Estimation Methods. Environmental Behavior of Organic Compounds. 16, 1-50. Lyman W.J., Reehl, W.F., and Rosenblatt, D.H. (eds). McGraw-Hill, New York, NY, USA.

(88) Threshold Limit Values Book 1993-1994.

(89) Toxigenics. (1981). 90-Day vapor inhalation study of methyl ethyl ketone in albino rats. Toxigenics' Study 420-0305. Toxigenics, Inc., 1800 East Pershing Road, Decatur, IL 62526.

(90) Wagner. 1974. Wasser, 42:271-305.

(91) World Health Organization. 1987. Environmental Health Criteria 65.

(92) Yonezawa, Y. and Urushigawa, Y. 1979. Chemosphere 8, 139-142.

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

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B206 PC_WATER_SOL_TAB
F001 520
F002 1
F003 14-11-2006
F004 CLGETTS1
F023 A36-003
F024 1
F007 A02-03
F008 P08-02
F009 330
F011 25
F020 P09-03: measured
F021 1992
F022 A03-02
F025 A01-03:  CAS No. 6863-58-7; sec-butyl ether
F030 C14-001
EOR
F001 520
F002 2
F003 14-11-2006
F004 CLGETTS1
F023 A36-003
F024 2
F007 A02-03
F008 P08-02
F009 327
F011 25
F020 P09-03: calculated
F021 2003
F022 A03-01
F025 A01-03:  CAS No. 6863-58-7; sec-butyl ether
F030 C14-001
EOB
C
B301 EN_PHOTODEGRADATION_TAB
F001 520
F002 1
F003 14-11-2006
F004 CLGETTS1
F045 A36-003
F046 2
F007 A01-03:  CAS No. 6863-58-7; sec-butyl ether
F008 F01-01
F009 F02-05:  Calculated values using AOPWIN version 1.91, a subroutine of the
*    computer program EPIWIN version 3.12
F010 2003
F011 F03-01
F034 F06-03
F035 1500000
F036 F07-02
F044 A02-03
F037 .000000000000320784
F043 A03-01
EOR
F001 520
F002 2
F003 14-11-2006
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F004 CLGETTS1
F046 1
F007 A01-03: CAS No. 6863-58-7; sec-butyl ether
F008 F01-04
F009 F02-05: Technical discussion
F010 2006
EOB
C
B302 EN_STABILITY_IN_WATER_TAB
F001 520
F002 1
F003 14-11-2006
F004 CLGETTS1
F041 1
F007 A01-03: CAS No. 6863-58-7; sec-butyl ether
F008 F08-01
F009 F09-03: technical discussion
F010 2006
EOB
C
B305 EN_TRANSPORT_TAB
F001 520
F002 1
F003 14-11-2006
F004 CLGETTS1
F011 A36-003
F012 1
F007 F20-07
F008 F22-01: air - sediment(s) - soil - water
F009 F21-01: Calculation according Mackay, Level III
F010 2006
EOR
F001 520
F002 2
F003 14-11-2006
F004 CLGETTS1
F011 A36-003
F012 2
F007 F20-05
F008 F22-01: air - biota - sediment(s) - soil - water
F009 F21-01: Calculation according Mackay, Level I
F010 2006
EOB
C
B308 EN_BIODEGRADATION_TAB
F001 520
F002 1
F003 14-11-2006
F004 CLGETTS1
F047 A36-003
F048 1
F007 A01-03: CAS No. 6863-58-7; sec-butyl ether
F008 F25-01
F009 F26-25: calculated using BIOWIN version 4.02
F010 2006
F020 F30-02: not readily biodegradable
F046 A03-01

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EOR
F001 520
F002 2
F003 14-11-2006
F004 CLGETTS1
F047 A36-003
F048 2
F007 A01-03:  CAS No. 6863-58-7; sec-butyl ether
F008 F25-01
F009 F26-25: Japanese Guideline by MITI (1974). Comparable to OECD TG 301C,
*    Modified MITI Test 1
F010 1992
F011 F27-0137
F012 100
F013 F28-02
F014 F29-03
F015 A02-03
F016 4
F017 3
F018 28
F019 F05-01
F020 F30-02: not readily biodegradable
F046 A03-02
EOB
C
B310 EN_BIOACCUMULATION_TAB
F001 520
F002 1
F003 14-11-2006
F004 CLGETTS1
F021 A36-003
F022 1
F007 A01-03:  CAS No. 6863-58-7; sec-butyl ether
F008 E02-0033
F009 F34-06: guideline corresponds to OECD 305C, Degree of Bioconcentration in
*    Fish (1981)
F011 42
F012 F10-01
F016 A02-03
F017 47
F018 83
F020 A03-02
EOR
F001 520
F002 2
F003 14-11-2006
F004 CLGETTS1
F021 A36-003
F022 2
F007 A01-03:  CAS No. 6863-58-7; sec-butyl ether
F009 F34-06: calculated
F010 2006
F016 A02-03
F017 32.1
F020 A03-01
EOB
C
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B401 EC_FISHTOX_TAB
F001 520
F002 1
F003 14-11-2006
F004 CLGETTS1
F033 A36-003
F034 1
F007 A01-03:  CAS No. 6863-58-7; sec-butyl ether
F008 E01-03: calculated
F009 E02-0161: freshwater fish
F010 E03-05: ECOSAR Computer Model
F011 2006
F012 96
F013 E04-02
F014 E05-02
F021 A02-03
F022 14.7
F045 E35-01
EOR
F001 520
F002 2
F003 14-11-2006
F004 CLGETTS1
F033 A36-003
F034 2
F007 A01-03:  CAS No. 6863-58-7; sec-butyl ether
F008 E01-03: calculated
F009 E02-0161: freshwater fish
F010 E03-05: ECOSAR Computer Model
F011 2006
F012 96
F013 E04-02
F014 E05-02
F021 A02-03
F022 10.8
F032 A03-01
F045 E35-01
EOR
F001 520
F002 3
F003 14-11-2006
F004 CLGETTS1
F033 A36-003
F034 3
F007 A01-03:  CAS No. 6863-58-7; sec-butyl ether
F008 E01-04
F009 E02-0106
F010 E03-05: Japanese Industrial Standard (JIS K 0102-1986-71): Testing
*    Methods for Industrial Wastewater.
F011 1992
F012 48
F013 E04-02
F014 E05-02
F021 A02-03
F022 30.7
F032 A03-02
F045 E35-02
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F050 C47-001
EOB
C
B402 EC_DAPHNIATOX_TAB
F001 520
F002 1
F003 14-11-2006
F004 CLGETTS1
F032 A36-003
F033 1
F007 A01-03: CAS No. 6863-58-7; sec-butyl ether
F008 E06-0013
F009 E07-04: ECOSAR Computer Model
F010 2006
F011 48
F012 E04-02
F013 E05-02
F020 A02-03
F021 16.7
F031 A03-01
F045 E35-01
EOR
F001 520
F002 2
F003 14-11-2006
F004 CLGETTS1
F032 A36-003
F033 2
F007 A01-03: CAS No. 6863-58-7; sec-butyl ether
F008 E06-0013
F009 E07-04: ECOSAR Computer Model
F010 2006
F011 48
F012 E04-02
F013 E05-02
F020 A02-03
F021 12.5
F031 A03-01
F045 E35-01
EOB
C
B403 EC_ALGAETOX_TAB
F001 520
F002 1
F003 14-11-2006
F004 CLGETTS1
F036 A36-003
F037 1
F007 A01-03: CAS No. 6863-58-7; sec-butyl ether
F008 E08-0063: green alga
F009 E09-04: ECOSAR Computer Model
F010 2006
F012 96
F013 E04-02
F014 E05-02
F027 A02-03
F028 11

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F035 A03-01
F050 E35-01
EOR
F001 520
F002 2
F003 14-11-2006
F004 CLGETTS1
F036 A36-003
F037 2
F007 A01-03:  CAS No. 6863-58-7; sec-butyl ether
F008 E08-0063: green alga
F009 E09-04: ECOSAR Computer Model
F010 2006
F012 96
F013 E04-02
F014 E05-02
F027 A02-03
F028 8.3
F035 A03-01
F050 E35-01
EOB
C
B405 EC_CHRONFISHTOX_TAB
F001 520
F002 1
F003 14-11-2006
F004 CLGETTS1
F030 A36-003
F031 1
F007 A01-03:  CAS No. 6863-58-7; sec-butyl ether
F008 E02-0161: Freshwater Fish (calculated toxicity values are not species
*    specific)
F009 E13-02: ECOSAR Computer Model
F010 2006
F011 E14-02: LC50
F012 30
F013 E15-01
F014 E05-02
F024 ChV
F025 A02-03
F026 2.2
F029 A03-01
F035 E35-01
EOR
F001 520
F002 2
F003 14-11-2006
F004 CLGETTS1
F030 A36-003
F031 2
F007 A01-03:  CAS No. 6863-58-7; sec-butyl ether
F008 E02-0161: Freshwater Fish (calculated toxicity values are not species
*    specific)
F009 E13-02: ECOSAR Computer Model
F010 2006
F011 E14-02: LC50
F012 30
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F013 E15-01
F014 E05-02
F024 ChV
F025 A02-03
F026 1.6
F029 A03-01
F035 E35-01
EOB
C
B406 EC_CHRONDAPHNIATOX_TAB
F001 520
F002 1
F003 14-11-2006
F004 CLGETTS1
F030 A36-003
F031 1
F007 A01-03:  CAS No. 6863-58-7; sec-butyl ether
F008 E06-0013
F009 E16-02: ECOSAR Computer model
F010 2006
F011 E17-01
F012 16
F013 E18-01
F014 E05-02
F015 A02-03
F016 1.3
F029 A03-01
F032 E35-01
EOR
F001 520
F002 2
F003 14-11-2006
F004 CLGETTS1
F030 A36-003
F031 2
F007 A01-03:  CAS No. 6863-58-7; sec-butyl ether
F008 E06-0013
F009 E16-02: ECOSAR Computer model
F010 2006
F011 E17-01
F012 16
F013 E18-01
F014 E05-02
F015 A02-03
F016 1
F029 A03-01
F032 E35-01
EOB
C
B601 TEXT_TAB
F002 520
F010 1.12
F004 1
F005 RM
F006 Search covered all Physical Chemical Properties, Environmental Fate,
*    Aquatic and Mammalian Toxicity endpoints related to the CAS number.
F007 Search covered all Physical Chemical Properties, Environmental Fate,
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*    Aquatic and Mammalian Toxicity endpoints related to the CAS number.
F020 260662
EOR
F002 520
F010 1.12
F004 2
F005 RM
F006 Search covered all Physical Chemical Properties, Environmental Fate,
*    Aquatic and Mammalian Toxicity endpoints related to the CAS number.
F007 Search covered all Physical Chemical Properties, Environmental Fate,
*    Aquatic and Mammalian Toxicity endpoints related to the CAS number.
F020 260663
EOR
F002 520
F010 1.12
F004 3
F005 RM
F006 Search covered all Physical Chemical Properties, Environmental Fate,
*    Aquatic and Mammalian Toxicity endpoints related to the CAS number.
F007 Search covered all Physical Chemical Properties, Environmental Fate,
*    Aquatic and Mammalian Toxicity endpoints related to the CAS number.
F020 260664
EOR
F002 520
F010 2.1
F004 1
F005 RE
F006 EPI SuiteTM (2000). Estimation Program Interface Suite, version 3.12.
*    Syracuse Research Corporation, Syracuse, NY, USA.
F007 EPI SuiteTM (2000). Estimation Program Interface Suite, version 3.12.
*    Syracuse Research Corporation, Syracuse, NY, USA.
F020 260558
EOR
F002 520
F010 2.1
F004 1
F005 RL
F006 Although the original data were not retrieved and reviewed for quality,
*    they were developed following acceptable test methods and therefore
*    considered reliable. Value was provided by the experimental database of
*    the EPIWIN program.
F007 Although the original data were not retrieved and reviewed for quality,
*    they were developed following acceptable test methods and therefore
*    considered reliable. Value was provided by the experimental database of
*    the EPIWIN program.
F020 260557
EOR
F002 520
F010 2.1
F004 1
F005 TS
F006 CAS No. 6863-58-7; sec-butyl ether
F007 CAS No. 6863-58-7; sec-butyl ether
F020 260546
EOR
F002 520
F010 2.1
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F004 2
F005 ME
F006 Calculated values using MPBPWIN version 1.41, a subroutine of the
* computer program EPIWIN version 3.12
F007 Calculated values using MPBPWIN version 1.41, a subroutine of the
* computer program EPIWIN version 3.12
F020 260573
EOR
F002 520
F010 2.1
F004 2
F005 RE
F006 EPI SuiteTM (2000). Estimation Program Interface Suite, version 3.12.
* Syracuse Research Corporation, Syracuse, NY, USA.
F007 EPI SuiteTM (2000). Estimation Program Interface Suite, version 3.12.
* Syracuse Research Corporation, Syracuse, NY, USA.
F020 260572
EOR
F002 520
F010 2.1
F004 2
F005 RL
F006 The result is a calculated value based on the chemical structure and
* represents a potential melting point for the substance with the CAS
* number listed under test substance.
F007 The result is a calculated value based on the chemical structure and
* represents a potential melting point for the substance with the CAS
* number listed under test substance.
F020 260575
EOR
F002 520
F010 2.1
F004 2
F005 TC
F006 Melting Point estimations performed by MPBPWIN are based on the average
* result of the calculation methods of K. Joback and Gold and Ogle.
**
** Joback's Method is described in Joback, K.G. 1982. A Unified Approach to
* Physical Property Estimation
F007 Melting Point estimations performed by MPBPWIN are based on the average
* result of the calculation methods of K. Joback and Gold and Ogle.
**
** Joback's Method is described in Joback, K.G. 1982. A Unified Approach to
* Physical Property Estimation Using Multivariate Statistical Techniques.
* In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid,
* J.M. Prausnitz and B.E. Poling, Eds.
**
** The Gold and Ogle Method simply uses the formula
** Tm = 0.5839Tb, where Tm is the melting point in Kelvin and Tb is the
* boiling point in Kelvin.
F020 260574
EOR
F002 520
F010 2.1
F004 2
F005 TS
F006 CAS No. 6863-58-7; sec-butyl ether

F007 CAS No. 6863-58-7; sec-butyl ether
F020 260571
EOR
F002 520
F010 2.2
F004 1
F005 RE
F006 EPI SuiteTM (2000). Estimation Program Interface Suite, version 3.12.
*   Syracuse Research Corporation, Syracuse, NY, USA.
F007 EPI SuiteTM (2000). Estimation Program Interface Suite, version 3.12.
*   Syracuse Research Corporation, Syracuse, NY, USA.
F020 260559
EOR
F002 520
F010 2.2
F004 1
F005 RL
F006 The result is a calculated value based on the chemical structure and
*   represents a potential boiling point for the substance with the CAS
*   number listed under test substance.
F007 The result is a calculated value based on the chemical structure and
*   represents a potential boiling point for the substance with the CAS
*   number listed under test substance.
F020 260561
EOR
F002 520
F010 2.2
F004 1
F005 TC
F006 Boiling point calculated by MPBPWIN subroutine, which is based on the
*   method of S. Stein and R. Brown in "Estimation of Normal Boiling Points
*   from Group Contributions". 1994. J. Chem. Inf. Comput. Sci. 34: 581-587.
F007 Boiling point calculated by MPBPWIN subroutine, which is based on the
*   method of S. Stein and R. Brown in "Estimation of Normal Boiling Points
*   from Group Contributions". 1994. J. Chem. Inf. Comput. Sci. 34: 581-587.
F020 260560
EOR
F002 520
F010 2.2
F004 1
F005 TS
F006 CAS No. 6863-58-7; sec-butyl ether
F007 CAS No. 6863-58-7; sec-butyl ether
F020 260547
EOR
F002 520
F010 2.3
F004 1
F005 RE
F006 Drake, Nathan L. (1935). Journal of the American Chemical Society. Vol
*   57, pp. 2623-2625 CAPLUS.
F007 Drake, Nathan L. (1935). Journal of the American Chemical Society. Vol
*   57, pp. 2623-2625 CAPLUS.
F020 260562
EOR
F002 520
F010 2.3

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F004 1
F005 RL
F006 Although the original data were not retrieved and reviewed for quality,
*    they were reported in the peer-reviewed literature and therefore
*    considered reliable.
F007 Although the original data were not retrieved and reviewed for quality,
*    they were reported in the peer-reviewed literature and therefore
*    considered reliable.
F020 260563
EOR
F002 520
F010 2.3
F004 1
F005 TS
F006 CAS No. 6863-58-7; sec-butyl ether
F007 CAS No. 6863-58-7; sec-butyl ether
F020 260548
EOR
F002 520
F010 2.4
F004 1
F005 RE
F006 EPI SuiteTM (2000). Estimation Program Interface Suite, version 3.12.
*    Syracuse Research Corporation, Syracuse, NY, USA.
F007 EPI SuiteTM (2000). Estimation Program Interface Suite, version 3.12.
*    Syracuse Research Corporation, Syracuse, NY, USA.
F020 260565
EOR
F002 520
F010 2.4
F004 1
F005 RL
F006 Although the original data were not retrieved and reviewed for quality,
*    they were developed following acceptable test methods and therefore
*    considered reliable. Value was provided by the experimental database of
*    the EPIWIN program.
**
**   Referen
F007 Although the original data were not retrieved and reviewed for quality,
*    they were developed following acceptable test methods and therefore
*    considered reliable. Value was provided by the experimental database of
*    the EPIWIN program.
**
**   Reference given in EPI Suite: Yaws, CL (1994B).
F020 260564
EOR
F002 520
F010 2.4
F004 1
F005 TS
F006 CAS No. 6863-58-7; sec-butyl ether
F007 CAS No. 6863-58-7; sec-butyl ether
F020 260549
EOR
F002 520
F010 2.4
F004 2
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F005 ME
F006 Vapor pressure calculation by MPBPWIN ver. 1.40 using calculation method
*   of Grain.
F007 Vapor pressure calculation by MPBPWIN ver. 1.40 using calculation method
*   of Grain.
F020 260567
EOR
F002 520
F010 2.4
F004 2
F005 RE
F006 EPI SuiteTM (2000). Estimation Program Interface Suite, version 3.12.
*   Syracuse Research Corporation, Syracuse, NY, USA.
F007 EPI SuiteTM (2000). Estimation Program Interface Suite, version 3.12.
*   Syracuse Research Corporation, Syracuse, NY, USA.
F020 260570
EOR
F002 520
F010 2.4
F004 2
F005 RL
F006 The result is a calculated value based on the chemical structure and
*   represents a potential vapor pressure for the substance with the CAS
*   number listed under test substance.
F007 The result is a calculated value based on the chemical structure and
*   represents a potential vapor pressure for the substance with the CAS
*   number listed under test substance.
F020 260569
EOR
F002 520
F010 2.4
F004 2
F005 RM
F006 EPIWIN is used and advocated by the US EPA for chemical property
*   estimation.
F007 EPIWIN is used and advocated by the US EPA for chemical property
*   estimation.
F020 260568
EOR
F002 520
F010 2.4
F004 2
F005 TS
F006 CAS No. 6863-58-7; sec-butyl ether
F007 CAS No. 6863-58-7; sec-butyl ether
F020 260566
EOR
F002 520
F010 2.5
F004 1
F005 RE
F006 Chemicals Inspection and Testing Institute (CITI) (1992). Biodegradation
*   and bioaccumulation data of existing chemicals based on the CSCL Japan.
*   CITI (ed.). Chemical Products Safety Division, Basic Industries Bureau,
*   Ministry of Internatio
F007 Chemicals Inspection and Testing Institute (CITI) (1992). Biodegradation
*   and bioaccumulation data of existing chemicals based on the CSCL Japan.

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*    CITI  (ed.). Chemical Products Safety Division, Basic Industries Bureau,
*    Ministry of International Trade and Industry, Japan. Japan Chemical
*    Industry Ecology-Toxicology and Information Center.
F020 260576
EOR
F002 520
F010 2.5
F004 1
F005 RL
F006 Although the original data were not retrieved and reviewed for quality,
*    they were developed at a well respected testing facility and therefore
*    considered reliable.
F007 Although the original data were not retrieved and reviewed for quality,
*    they were developed at a well respected testing facility and therefore
*    considered reliable.
F020 260583
EOR
F002 520
F010 2.5
F004 1
F005 TC
F006 Specific methods were not given in the document reporting the measured
*    value.  Measurements were performed at the Chemicals Inspection and
*    Testing Institute of Japan.
F007 Specific methods were not given in the document reporting the measured
*    value.  Measurements were performed at the Chemicals Inspection and
*    Testing Institute of Japan.
F020 260582
EOR
F002 520
F010 2.5
F004 1
F005 TS
F006 CAS No. 6863-58-7; sec-butyl ether
F007 CAS No. 6863-58-7; sec-butyl ether
F020 260550
EOR
F002 520
F010 2.5
F004 2
F005 ME
F006 Calculated values using KOWWIN version 1.67, a subroutine of the computer
*    program EPIWIN version 3.12
F007 Calculated values using KOWWIN version 1.67, a subroutine of the computer
*    program EPIWIN version 3.12
F020 260578
EOR
F002 520
F010 2.5
F004 2
F005 RE
F006 EPI SuiteTM (2000). Estimation Program Interface Suite, version 3.12.
*    Syracuse Research Corporation, Syracuse, NY, USA.
F007 EPI SuiteTM (2000). Estimation Program Interface Suite, version 3.12.
*    Syracuse Research Corporation, Syracuse, NY, USA.
F020 260581
EOR
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F002 520
F010 2.5
F004 2
F005 RL
F006 The result is a calculated value based on the chemical structure and
*   represents a potential partition coefficient for the substance with the
*   CAS number listed under test substance.
F007 The result is a calculated value based on the chemical structure and
*   represents a potential partition coefficient for the substance with the
*   CAS number listed under test substance.
F020 260580
EOR
F002 520
F010 2.5
F004 2
F005 TC
F006 Octanol / Water Partition Coefficient estimations performed by KOWWIN are
*   based on an atom/fragment contribution method of W. Meylan and P. Howard
*   in "Atom/fragment contribution method for estimating octanol-water
*   partition coefficients". 1
F007 Octanol / Water Partition Coefficient estimations performed by KOWWIN are
*   based on an atom/fragment contribution method of W. Meylan and P. Howard
*   in "Atom/fragment contribution method for estimating octanol-water
*   partition coefficients". 1995. J. Pharm. Sci. 84:83-92.
F020 260579
EOR
F002 520
F010 2.5
F004 2
F005 TS
F006 CAS No. 6863-58-7; sec-butyl ether
F007 CAS No. 6863-58-7; sec-butyl ether
F020 260577
EOR
F002 520
F010 2.6.1
F004 1
F005 RE
F006 Chemicals Inspection and Testing Institute (CITI) (1992). Biodegradation
*   and bioaccumulation data of existing chemicals based on the CSCL Japan.
*   CITI (ed.). Chemical Products Safety Division, Basic Industries Bureau,
*   Ministry of Internatio
F007 Chemicals Inspection and Testing Institute (CITI) (1992). Biodegradation
*   and bioaccumulation data of existing chemicals based on the CSCL Japan.
*   CITI (ed.). Chemical Products Safety Division, Basic Industries Bureau,
*   Ministry of International Trade and Industry, Japan. Japan Chemical
*   Industry Ecology-Toxicology and Information Center.
F020 260584
EOR
F002 520
F010 2.6.1
F004 1
F005 RL
F006 Although the original data were not retrieved and reviewed for quality,
*   they were developed at a well respected testing facility and therefore
*   considered reliable.
F007 Although the original data were not retrieved and reviewed for quality,

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*    they were developed at a well respected testing facility and therefore
*    considered reliable.
F020 260585
EOR
F002 520
F010 2.6.1
F004 1
F005 TC
F006 Specific methods were not given in the document reporting the measured
*    value.  Measurements were performed at the Chemicals Inspection and
*    Testing Institute of Japan.
F007 Specific methods were not given in the document reporting the measured
*    value.  Measurements were performed at the Chemicals Inspection and
*    Testing Institute of Japan.
F020 260586
EOR
F002 520
F010 2.6.1
F004 1
F005 TS
F006 CAS No. 6863-58-7; sec-butyl ether
F007 CAS No. 6863-58-7; sec-butyl ether
F020 260551
EOR
F002 520
F010 2.6.1
F004 2
F005 ME
F006 Calculated values using WSKOWWIN version 1.41, a subroutine of the
*    computer program EPIWIN version 3.12
F007 Calculated values using WSKOWWIN version 1.41, a subroutine of the
*    computer program EPIWIN version 3.12
F020 260588
EOR
F002 520
F010 2.6.1
F004 2
F005 RE
F006 EPI SuiteTM (2000). Estimation Program Interface Suite, version 3.12.
*    Syracuse Research Corporation, Syracuse, NY, USA.
F007 EPI SuiteTM (2000). Estimation Program Interface Suite, version 3.12.
*    Syracuse Research Corporation, Syracuse, NY, USA.
F020 260591
EOR
F002 520
F010 2.6.1
F004 2
F005 RL
F006 The result is a calculated value based on the chemical structure and
*    represents a potential water solubility for the substance with the CAS
*    number listed under test substance.
F007 The result is a calculated value based on the chemical structure and
*    represents a potential water solubility for the substance with the CAS
*    number listed under test substance.
F020 260590
EOR
F002 520
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F010 2.6.1
F004 2
F005 TC
F006 Water Solubility estimations performed by WSKOWWIN are based on a Kow
*   correlation method described by W. Meylan, P. Howard and R. Boethling in
*   "Improved method for estimating water solubility from octanol/water
*   partition coefficient". Envir
F007 Water Solubility estimations performed by WSKOWWIN are based on a Kow
*   correlation method described by W. Meylan, P. Howard and R. Boethling in
*   "Improved method for estimating water solubility from octanol/water
*   partition coefficient". Environ. Toxicol. Chem. 15:100-106. 1995.
F020 260589
EOR
F002 520
F010 2.6.1
F004 2
F005 TS
F006 CAS No. 6863-58-7; sec-butyl ether
F007 CAS No. 6863-58-7; sec-butyl ether
F020 260587
EOR
F002 520
F010 3.1.1
F004 1
F005 RE
F006 EPI SuiteTM (2000). Estimation Program Interface Suite, version 3.12.
*   Syracuse Research Corporation, Syracuse, NY, USA.
F007 EPI SuiteTM (2000). Estimation Program Interface Suite, version 3.12.
*   Syracuse Research Corporation, Syracuse, NY, USA.
F020 260593
EOR
F002 520
F010 3.1.1
F004 1
F005 RL
F006 The results include calculated data based on chemical structure as
*   modeled by AOPWIN. The data represent a potential atmospheric half-life
*   range for the test substance.
F007 The results include calculated data based on chemical structure as
*   modeled by AOPWIN. The data represent a potential atmospheric half-life
*   range for the test substance.
F020 260596
EOR
F002 520
F010 3.1.1
F004 1
F005 RS
F006 Atmospheric Oxidation Potential
**
**   In the environment, organic chemicals emitted into the troposphere are
*   degraded by several important transformation processes. The dominant
*   transformation process for most compounds is the daylight reaction
F007 Atmospheric Oxidation Potential
**
**   In the environment, organic chemicals emitted into the troposphere are
*   degraded by several important transformation processes. The dominant
*   transformation process for most compounds is the daylight reaction with

```
*    hydroxyl (OH-) radicals (Atkinson, 1988, 1989). The rate at which an
*    organic compound reacts with OH- radicals is a direct measure of its
*    atmospheric persistence (Meylan and Howard, 1993).
**
**   AOPWIN estimates the rate constant for the atmospheric, gas-phase
*    reaction between photochemically produced hydroxyl radicals and organic
*    chemicals.  The rate constants estimated by the program are then used to
*    calculate atmospheric half-lives for organic compounds based upon average
*    atmospheric concentrations of hydroxyl radicals.
**
**   Since the reactions only take place in the presence of sunlight, the
*    atmospheric half-lives are normalized for a 12-hour day.
**
**
**   Calculated*        OH- Rate Constant
**   half-life (days)         (cm3/molecule-sec)
**
**   0.333              32.0784 E-12
**
**
**   References:
**
**   Atkinson, R. 1988. Estimation of gas-phase hydroxyl radical rate
*    constants for organic chemicals. Environ. Toxicol. Chem. 7:435-442.
**
**   Atkinson, R. 1989. Kinetics and mechanisms of the gas-phase reactions of
*    the hydroxyl radical with organic compounds. J. Phys. Chem. Ref. Data
*    Monograph No. 1, Amer. Inst. Physics & Amer. Chem. Soc., NY.
**
**   Meylan, W.M. and P.H. Howard. 1993.  Computer estimation of the
*    atmospheric gas-phase reaction rate of organic compounds with hydroxyl
*    radicals and ozone. Chemosphere 12:2293-2299.
F020 260594
EOR
F002 520
F010 3.1.1
F004 1
F005 TC
F006
**   Indirect photodegradation, or atmospheric oxidation potential, is based
*    on the structure-activity relationship methods developed by R. Atkinson.
**
**   Temperature: 25°C
**   Sensitizer:  OH radical
**   Concentration of Sensitizer:   1.5 E6 OH radicals/cm3
F007
**   Indirect photodegradation, or atmospheric oxidation potential, is based
*    on the structure-activity relationship methods developed by R. Atkinson.
**
**   Temperature: 25°C
**   Sensitizer:  OH radical
**   Concentration of Sensitizer:   1.5 E6 OH radicals/cm3
**
F020 260595
EOR
F002 520
F010 3.1.1
```

```
F004 1
F005 TS
F006 CAS No. 6863-58-7; sec-butyl ether
F007 CAS No. 6863-58-7; sec-butyl ether
F020 260592
EOR
F002 520
F010 3.1.1
F004 2
F005 RE
F006 EMBSI (2006) Photodegradation (Direct): CAS No. 6863-58-7; sec-Butyl
*    Ether.
F007 EMBSI (2006) Photodegradation (Direct): CAS No. 6863-58-7; sec-Butyl
*    Ether.
F020 260599
EOR
F002 520
F010 3.1.1
F004 2
F005 RS
F006 Photolysis as a Function of Molecular Structure
**
**   The direct photolysis of an organic molecule occurs when it absorbs
*    sufficient light energy to result in a structural transformation (Harris,
*    1982). The reaction process is initiated when lig
F007 Photolysis as a Function of Molecular Structure
**
**   The direct photolysis of an organic molecule occurs when it absorbs
*    sufficient light energy to result in a structural transformation (Harris,
*    1982). The reaction process is initiated when light energy in a specific
*    wavelength range elevates a molecule to an electronically excited state.
*    However, the excited state is competitive with various deactivation
*    processes that can result in the return of the molecule to a non excited
*    state.
**
**   The absorption of light in the ultra violet (UV)-visible range, 110-750
*    nm, can result in the electronic excitation of an organic molecule. Light
*    in this range contains energy of the same order of magnitude as covalent
*    bond dissociation energies (Harris, 1982). Higher wavelengths (e.g.
*    infrared) result only in vibrational and rotational transitions, which do
*    not tend to produce structural changes to a molecule.
**
**   The stratospheric ozone layer prevents UV light of less than 290 nm from
*    reaching the earth's surface. Therefore, only light at wavelengths
*    between 290 and 750 nm can result in photochemical transformations in the
*    environment (Harris, 1982). Although the absorption of UV light in the
*    290-750 nm range is necessary, it is not always sufficient for a chemical
*    to undergo photochemical degradation. Energy may be re-emitted from an
*    excited molecule by mechanisms other than chemical transformation,
*    resulting in no change to the parent molecule.
**
**   A conservative approach to estimating a photochemical degradation rate is
*    to assume that degradation will occur in proportion to the amount of
*    light wavelengths >290 nm absorbed by the molecule (Zepp and Cline,
*    1977).
**
**   Saturated hydrocarbons and R-OH groups do not absorb light above 290 nm
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*    (Harris J, 1982a).  Therefore, these moieties are stable in regard to
*    direct photolytic processes. Ethers are also stable as this group absorbs
*    UV light in the far UV region, below 220 nm (Mill T, 2000), therefore,
*    direct photolysis will not be an important transformation process for the
*    degradation of sec-butyl ether in the environment.
**
**   References:
**
**   Harris, J. C. 1982. "Rate of Aqueous Photolysis," Chapter 8 in: W. J.
*    Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical
*    Property Estimation Methods, McGraw-Hill Book Company, New York, USA.
**
**   Zepp, R. G. and D. M. Cline. 1977. Rates of Direct Photolysis in the
*    Aqueous Environment, Environ. Sci. Technol., 11:359-366.
**
**   Boethling, R.S., Mackay, D. 2000.  Handbook of Property Estimation
*    Methods for Chemicals, CRC Press, Boca Raton, FL, USA.
F020 260598
EOR
F002 520
F010 3.1.1
F004 2
F005 TS
F006 CAS No. 6863-58-7; sec-butyl ether
F007 CAS No. 6863-58-7; sec-butyl ether
F020 260597
EOR
F002 520
F010 3.1.2
F004 1
F005 RE
F006 EMBSI (2006) Hydrolysis: CAS No. 6863-58-7; sec-Butyl Ether.
F007 EMBSI (2006) Hydrolysis: CAS No. 6863-58-7; sec-Butyl Ether.
F020 260602
EOR
F002 520
F010 3.1.2
F004 1
F005 RS
F006 Hydrolysis as a Function of Molecular Structure
**
**   Hydrolysis of an organic molecule occurs when a molecule (R-X) reacts
*    with water (H2O) to form a new carbon-oxygen bond after the carbon-X bond
*    is cleaved (Gould, 1959; Harris, 1982). Mechani
F007 Hydrolysis as a Function of Molecular Structure
**
**   Hydrolysis of an organic molecule occurs when a molecule (R-X) reacts
*    with water (H2O) to form a new carbon-oxygen bond after the carbon-X bond
*    is cleaved (Gould, 1959; Harris, 1982). Mechanistically, this reaction is
*    referred to as a nucleophilic substitution reaction, where X is the
*    leaving group being replaced by the incoming nucleophilic oxygen from the
*    water molecule.
**
**   Chemicals that are susecptible to hydrolysis contain functional groups
*    that can be displaced by a nucleophilic substitution reaction. Substances
*    that have a potential to hydrolyze include alkyl halides, amides,
*    carbamates, carboxylic acid esters and lactones, epoxides, phosphate
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*    esters, and sulfonic acid esters (Neely, 1985). The lack of a suitable
*    leaving group renders a compound resistant to hydrolysis.
**
**   Sec-butyl ether is expected to be resistant to hydrolysis because it
*    lacks a functional group that is hydrolytically reactive (Harris, 1982b).
*     Therefore, hydrolysis will not contribute to its removal from the
*    environment.
**
**   References:
**
**   Gould, E.S. (1959), Mechanism and Structure in Organic Chemistry, Holt,
*    Reinhart and Winston, New York, NY, USA.
**
**   Harris, J.C. (1982), "Rate of Hydrolysis," Chapter 7 in: W.J. Lyman, W.F.
*    Reehl, and D.H. Rosenblatt, eds., Handbook of Chemical Property
*    Estimation Methods, McGraw-Hill Book Company, New York, NY, USA.
**
**   Neely, W. B. 1985. Hydrolysis. In: W. B. Neely and G. E. Blau, eds.
*    Environmental Exposure from Chemicals. Vol I., pp. 157-173. CRC Press,
*    Boca Raton, FL, USA.
F020 260601
EOR
F002 520
F010 3.1.2
F004 1
F005 TS
F006 CAS No. 6863-58-7; sec-butyl ether
F007 CAS No. 6863-58-7; sec-butyl ether
F020 260600
EOR
F002 520
F010 3.3.1
F004 1
F005 ME
F006 The EQC Level III model is a steady state model that is useful for
*    determining how the medium of release affects environmental fate.  Level
*    III fugacity allows non-equilibrium conditions to exist between connected
*    media as steady state, and
F007 The EQC Level III model is a steady state model that is useful for
*    determining how the medium of release affects environmental fate.  Level
*    III fugacity allows non-equilibrium conditions to exist between connected
*    media as steady state, and illustrate important transport and
*    transformation processes.
**
**   Physicochemical input values for the model were calculated using the
*    EPIWIN Estimation v 3.12 program.  Measured input values were also used
*    where available and obtained from the EPIWIN database or other reliable
*    sources. Distribution data from the equilibrium model provide basic
*    information on the potential partitioning behavior of chemicals between
*    selected environmental compartments (i.e., air, water, soil, and
*    sediment).
**
**   Input values used:
**   Molecular mass = 130.23 g/mol
**   Water solubility = 327 mg/L
**   Vapour pressure = 2170 Pa
**   log Kow = 2.87
```

```
**   Melting point = -100 deg C
**
**   Degradation half-lives:
**
**   Air - 4.0 hrs
**   Water - 360 hrs
**   Soil - 7200 hrs
**   Sediment - 72000 hrs
**
**   This model was run assuming the default emissions.
F020 260603
EOR
F002 520
F010 3.3.1
F004 1
F005 RE
F006 Mackay D, DiGuardo A, Paterson S and Cowan C (2003). EQC Model ver. 2.02,
*    available from the Environmental Centre, Trent University, Canada.
F007 Mackay D, DiGuardo A, Paterson S and Cowan C (2003). EQC Model ver. 2.02,
*    available from the Environmental Centre, Trent University, Canada.
F020 260606
EOR
F002 520
F010 3.3.1
F004 1
F005 RL
F006 This robust summary has a reliability rating of 2 because the data are
*    calculated and not measured.
F007 This robust summary has a reliability rating of 2 because the data are
*    calculated and not measured.
F020 260605
EOR
F002 520
F010 3.3.1
F004 1
F005 RS
F006 Air - 3.2%
**   Water - 44.8%
**   Soil - 51.1%
**   Sediment - 0.9%
F007 Air - 3.2%
**   Water - 44.8%
**   Soil - 51.1%
**   Sediment - 0.9%
F020 260604
EOR
F002 520
F010 3.3.1
F004 1
F005 TS
F006 CAS No. 6863-58-7; sec-butyl ether
F007 CAS No. 6863-58-7; sec-butyl ether
F020 260552
EOR
F002 520
F010 3.3.1
F004 2
```

F005 ME
F006 The EQC Level I is a steady state, equilibrium model that utilizes the
*   input of basic chemical properties including molecular weight, vapor
*   pressure, and water solubility to calculate distribution within a
*   standardized regional environment.
F007 The EQC Level I is a steady state, equilibrium model that utilizes the
*   input of basic chemical properties including molecular weight, vapor
*   pressure, and water solubility to calculate distribution within a
*   standardized regional environment.
**
**   Physicochemical input values for the model were calculated using the
*   EPIWIN Estimation v 3.12 program. Measured input values were also used
*   where available and obtained from the EPIWIN database or other reliable
*   sources. Distribution data from the equilibrium model provide basic
*   information on the potential partitioning behavior of chemicals between
*   selected environmental compartments (i.e., air, water, soil, and
*   sediment).
**
**   Input values used:
**   Molecular mass = 130.23 g/mol
**   Water solubility = 327 mg/L
**   Vapour pressure = 2170 Pa
**   log Kow = 2.87
**   Melting point = -100 deg C
F020 260608
EOR
F002 520
F010 3.3.1
F004 2
F005 RE
F006 Mackay D, DiGuardo A, Paterson S and Cowan C (2003). EQC Model ver. 2.02,
*   available from the Environmental Centre, Trent University, Canada.
F007 Mackay D, DiGuardo A, Paterson S and Cowan C (2003). EQC Model ver. 2.02,
*   available from the Environmental Centre, Trent University, Canada.
F020 260607
EOR
F002 520
F010 3.3.1
F004 2
F005 RL
F006 This robust summary has a reliability rating of 2 because the data are
*   calculated and not measured.
F007 This robust summary has a reliability rating of 2 because the data are
*   calculated and not measured.
F020 260610
EOR
F002 520
F010 3.3.1
F004 2
F005 RS
F006 Air - 99.1%
**   Water - 0.5%
**   Soil - 0.4%
**   Sediment - <0.01%
**   Suspended Sed - <0.01%
**   Biota - <0.01%
F007 Air - 99.1%

**   Water - 0.5%
**   Soil - 0.4%
**   Sediment - <0.01%
**   Suspended Sed - <0.01%
**   Biota - <0.01%
F020 260609
EOR
F002 520
F010 3.3.1
F004 2
F005 TS
F006 CAS No. 6863-58-7; sec-butyl ether
F007 CAS No. 6863-58-7; sec-butyl ether
F020 260553
EOR
F002 520
F010 3.5
F004 1
F005 RE
F006 EPI SuiteTM (2000). Estimation Program Interface Suite, version 3.12.
*   Syracuse Research Corporation, Syracuse, NY, USA.
F007 EPI SuiteTM (2000). Estimation Program Interface Suite, version 3.12.
*   Syracuse Research Corporation, Syracuse, NY, USA.
F020 260673
EOR
F002 520
F010 3.5
F004 1
F005 RE
F006 Howard, PH, Boethling, RS, Stitler, WM, Meylan, WM, Hueber, AE, Beauman,
*   JA and Larosche, ME (1992). Predictive model for aerobic
*   biodegradability developed from a file of evaluated biodegradation data.
*   Environ Toxicol Chem 11, 593-603.
F007 Howard, PH, Boethling, RS, Stitler, WM, Meylan, WM, Hueber, AE, Beauman,
*   JA and Larosche, ME (1992). Predictive model for aerobic
*   biodegradability developed from a file of evaluated biodegradation data.
*   Environ Toxicol Chem 11, 593-603.
F020 260674
EOR
F002 520
F010 3.5
F004 1
F005 RL
F006 The value was calculated based on the chemical structure as modeled by
*   EPI Suite. This robust summary has a reliability rating of 2 because the
*   data are modeled.
F007 The value was calculated based on the chemical structure as modeled by
*   EPI Suite. This robust summary has a reliability rating of 2 because the
*   data are modeled.
F020 260672
EOR
F002 520
F010 3.5
F004 1
F005 RM
F006 Calculation of biodegradation and the timeframe for Primary and Ultimate
*   biodegradation using BIOWIN version 4.02, a subroutine of the computer

```
*    program EPI Suite version 3.12 as described by Howard, et al, 1994.
**
**   BIOWIN contains six models
F007 Calculation of biodegradation and the timeframe for Primary and Ultimate
*    biodegradation using BIOWIN version 4.02, a subroutine of the computer
*    program EPI Suite version 3.12 as described by Howard, et al, 1994.
**
**   BIOWIN contains six models (linear regression (BIOWIN 1), non-linear
*    regression (BIOWIN 2), ultimate degradation to CO2 and H2O (BIOWIN 3),
*    primary degradation (BIOWIN 4), linear regression estimate of the
*    probability of passing the OECD 301C / MITI-1 ready biodegradation test
*    (BIOWIN 5), and non-linear regression estimate of the probability of
*    passing the OECD 301C / MITI-1 ready biodegradation test (BIOWIN 6).
**
**   BIOWIN 1 - "Does Not Biodegrade Fast"
**   BIOWIN 2 - "Does Not Biodegrade Fast"
**   BIOWIN 3 - "Weeks"
**   BIOWIN 4 - "Days-Weeks"
**   BIOWIN 5 - "Does Not Biodegrade Fast"
**   BIOWIN 6 - "Does Not Biodegrade Fast"
**
**   According to the USEPA, BIOWIN 6 is better predictor of whether a
*    chemical will pass or fail the OECD 301C / MITI-1 ready biodegradation
*    test than BIOWIN 5.
F020 260671
EOR
F002 520
F010 3.5
F004 1
F005 TS
F006 CAS No. 6863-58-7; sec-butyl ether
F007 CAS No. 6863-58-7; sec-butyl ether
F020 260670
EOR
F002 520
F010 3.5
F004 2
F005 ME
F006 The test was conducted in accordance with "Biodegradation test of
*    chemical substances by microorganisms etc". stipulated in the Order
*    Prescribing the Items of the Test Relating to the New Chemical Substance
*    (1974, Order of the Prime Ministe
F007 The test was conducted in accordance with "Biodegradation test of
*    chemical substances by microorganisms etc". stipulated in the Order
*    Prescribing the Items of the Test Relating to the New Chemical Substance
*    (1974, Order of the Prime Minister, the Minister of Health and Welfare,
*    the Minister of International Trade and Industry No 1). This guideline
*    coresponds to "301C, Ready Biodegradability: Modified MITI Test 1"
*    stipulated in the OECD Guidelines for Testing of Chemicals (1981).
F020 260677
EOR
F002 520
F010 3.5
F004 2
F005 RE
F006 Chemicals Inspection and Testing Institute (CITI) (1992). Biodegradation
*    and bioaccumulation data of existing chemicals based on the CSCL Japan.
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*    CITI  (ed.). Chemical Products Safety Division, Basic Industries Bureau,
*    Ministry of Internatio
F007 Chemicals Inspection and Testing Institute (CITI) (1992). Biodegradation
*    and bioaccumulation data of existing chemicals based on the CSCL Japan.
*    CITI  (ed.). Chemical Products Safety Division, Basic Industries Bureau,
*    Ministry of International Trade and Industry, Japan. Japan Chemical
*    Industry Ecology-Toxicology and Information Center.
F020 260676
EOR
F002 520
F010 3.5
F004 2
F005 RL
F006 Although a standard method was not followed, the testing procedures
*    followed generally accepted aerobic biodegradation guideline methods and
*    although there was limited information on the specifics of the study,
*    there was sufficient informat
F007 Although a standard method was not followed, the testing procedures
*    followed generally accepted aerobic biodegradation guideline methods and
*    although there was limited information on the specifics of the study,
*    there was sufficient information on testing method and conditions in
*    general to rate this study a 2.
F020 260679
EOR
F002 520
F010 3.5
F004 2
F005 TC
F006 Sludge concentration = 30 mg/l
F007 Sludge concentration = 30 mg/l
F020 260678
EOR
F002 520
F010 3.5
F004 2
F005 TS
F006 Analogue substance CAS No. 142-96-1; n-butyl ether
F007 Analogue substance CAS No. 142-96-1; n-butyl ether
F020 260675
EOR
F002 520
F010 3.7
F004 1
F005 RE
F006 Chemicals Inspection and Testing Institute (CITI) (1992). Biodegradation
*    and bioaccumulation data of existing chemicals based on the CSCL Japan.
*    CITI  (ed.). Chemical Products Safety Division, Basic Industries Bureau,
*    Ministry of Internatio
F007 Chemicals Inspection and Testing Institute (CITI) (1992). Biodegradation
*    and bioaccumulation data of existing chemicals based on the CSCL Japan.
*    CITI  (ed.). Chemical Products Safety Division, Basic Industries Bureau,
*    Ministry of International Trade and Industry, Japan. Japan Chemical
*    Industry Ecology-Toxicology and Information Center.
F020 260544
EOR
F002 520
F010 3.7
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F004 1
F005 RL
F006 Although a standard method was not followed, the testing procedures
* followed generally accepted fish bioconcentration guideline methods and
* although there was limited information on the specifics of the study,
* there was sufficient informati
F007 Although a standard method was not followed, the testing procedures
* followed generally accepted fish bioconcentration guideline methods and
* although there was limited information on the specifics of the study,
* there was sufficient information on testing method and conditions in
* general to rate this study a 2.
F020 260545
EOR
F002 520
F010 3.7
F004 1
F005 RS
F006 At a concentration of 0.2 mg/L sec-butyl ether was shown to have
* bioconcentrate factor (BCF) range of 47 to 83, which is a log BCF range
* of 1.67 to 1.92.
**
** At a concentration of 0.02 mg/L sec-butyl ether was shown to have a BCF
* range of 30
F007 At a concentration of 0.2 mg/L sec-butyl ether was shown to have
* bioconcentrate factor (BCF) range of 47 to 83, which is a log BCF range
* of 1.67 to 1.92.
**
** At a concentration of 0.02 mg/L sec-butyl ether was shown to have a BCF
* range of 30 to 114, which is a log BCF range of 1.48 to 2.06.
F020 260543
EOR
F002 520
F010 3.7
F004 1
F005 TC
F006 Fish supplier was Sugishima fish farm, Kumamoto, Japan. Upon arrival,
* fish were placed in an acclimation tank with a flow through water system
* for 28 days at 25° +/-2° C. Test fish were then transferred to test tanks
* and reared again at the
F007 Fish supplier was Sugishima fish farm, Kumamoto, Japan. Upon arrival,
* fish were placed in an acclimation tank with a flow through water system
* for 28 days at 25° +/-2° C. Test fish were then transferred to test tanks
* and reared again at the same temperature for approximately 1 month.
**
** At test initiation, average fish weight, length, and lipid content were,
* 30 g, 10 cm, and 2-5%, respectively. Fish were fed pelleted feed for carp
* supplied by Haigo Shiryo K.K..
**
** Fish were fed approximately 2% of their total body weight daily. On days
* fish were sampled, they were not fed.
** The test systems included 100 L volume glass tanks with a flow ate of 200
* to 800 ml/min at 25° +/-2° C. Dissolved oxygen was 6 to 8 mg/L. At test
* initiation there was a minimum of 15 fish per exposure level. Treatment
* levels were based on results of acute toxicity testing.
**
** Test water, test fish, and control fish were analyzed twice a week, every
* two weeks, and prior to test initiation as well as at termination,

```
*    respectively. Recovery efficiency was determined in water and fish
*    homogenate. Analytical results from the definitive studies were corrected
*    based on efficiency results.
**
**   Bioconcentration factors were calculated based on:
**   test substance concentration in fish / test substance concentration in
*    water.
**
**   Two concentrations were evaluated: 0.2 mg/L and 0.02 mg/L.
**
**
F020 260542
EOR
F002 520
F010 3.7
F004 1
F005 TS
F006 Analogue substance CAS No. 142-96-1; n-butyl ether
F007 Analogue substance CAS No. 142-96-1; n-butyl ether
F020 260541
EOR
F002 520
F010 3.7
F004 2
F005 ME
F006 Calculated values using BCFWIN version 2.15, a subroutine of the computer
*    program EPIWIN version 3.12.
F007 Calculated values using BCFWIN version 2.15, a subroutine of the computer
*    program EPIWIN version 3.12.
F020 260634
EOR
F002 520
F010 3.7
F004 2
F005 RE
F006 EPI SuiteTM (2000). Estimation Program Interface Suite, version 3.12.
*    Syracuse Research Corporation, Syracuse, NY, USA.
F007 EPI SuiteTM (2000). Estimation Program Interface Suite, version 3.12.
*    Syracuse Research Corporation, Syracuse, NY, USA.
F020 260637
EOR
F002 520
F010 3.7
F004 2
F005 RL
F006 The result is a calculated value based on the chemical structure and
*    represents a potential bioaccumulation factor for the substance with the
*    CAS number listed under test substance.
F007 The result is a calculated value based on the chemical structure and
*    represents a potential bioaccumulation factor for the substance with the
*    CAS number listed under test substance.
F020 260636
EOR
F002 520
F010 3.7
F004 2
F005 TC
```

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F006
**   BCFWIN estimates the bioconcentration factor (BCF) of an organic compound
*    using the compound's log octanol-water partition coefficient (Kow).
**
**   The estimation methodology used by BCFWIN is described in "Improved
*    Method for Estimating Biocon
F007
**   BCFWIN estimates the bioconcentration factor (BCF) of an organic compound
*    using the compound's log octanol-water partition coefficient (Kow).
**
**   The estimation methodology used by BCFWIN is described in "Improved
*    Method for Estimating Bioconcentration Factor (BCF) from Octanol-Water
*    Partition Coefficient", SRC TR-97-006 (2nd Update), July 22, 1997.
**
**   Log Kow used = 2.87
**
**
**   Estimated BCF = 32.1
**   Estimated Log BCF = 1.507
**
F020 260635
EOR
F002 520
F010 3.7
F004 2
F005 TS
F006 CAS No. 6863-58-7; sec-butyl ether
F007 CAS No. 6863-58-7; sec-butyl ether
F020 260633
EOR
F002 520
F010 4.1
F004 1
F005 CL
F006 Based on the calculated Kow value of 2.87, sec-Butyl Ether is expected to
*    have an acute 96-hour LC50 of 14.7 mg/L and a Chronic Value of 2.2 mg/L
F007 Based on the calculated Kow value of 2.87, sec-Butyl Ether is expected to
*    have an acute 96-hour LC50 of 14.7 mg/L and a Chronic Value of 2.2 mg/L
F020 260612
EOR
F002 520
F010 4.1
F004 1
F005 RE
F006 Cash G and Nabholz V (1999). ECOSAR Classes for Microsoft Windows, ECOWIN
*    v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment
*    Division. Washington, DC, USA.
F007 Cash G and Nabholz V (1999). ECOSAR Classes for Microsoft Windows, ECOWIN
*    v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment
*    Division. Washington, DC, USA.
F020 260614
EOR
F002 520
F010 4.1
F004 1
F005 RL
F006 The value was calculated based on chemical structure as modeled by
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*    EPIWIN.  This robust summary has a reliability rating of 2 because the
*    data are calculated and not measured.
F007 The value was calculated based on chemical structure as modeled by
*    EPIWIN.  This robust summary has a reliability rating of 2 because the
*    data are calculated and not measured.
F020 260613
EOR
F002 520
F010 4.1
F004 1
F005 TC
F006 Log Kow (octanol/water partition coefficient) values and a chemical
*    structure are needed to calculate aquatic toxicity using the ECOSAR
*    model.  The Kow calculation is performed by KOWWIN based on an
*    atom/fragment contribution method of Meyl
F007 Log Kow (octanol/water partition coefficient) values and a chemical
*    structure are needed to calculate aquatic toxicity using the ECOSAR
*    model.  The Kow calculation is performed by KOWWIN based on an
*    atom/fragment contribution method of Meylan and Howard (1), which is a
*    subroutine in the EPISuite computer model (2).
**
**
**   1.  Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for
*    estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.
**
**   2.  EPI SuiteTM (2000). Estimation Program Interface Suite, version 3.12.
*    Syracuse Research Corporation, Syracuse, NY, USA.
F020 260611
EOR
F002 520
F010 4.1
F004 1
F005 TS
F006 CAS No. 6863-58-7; sec-butyl ether
F007 CAS No. 6863-58-7; sec-butyl ether
F020 260554
EOR
F002 520
F010 4.1
F004 2
F005 CL
F006 Based on the calculated Kow value of 3.01, n-Butyl Ether is expected to
*    have an acute 96-hour LC50 of 10.8 mg/L and a Chronic Value of 1.6 mg/L.
F007 Based on the calculated Kow value of 3.01, n-Butyl Ether is expected to
*    have an acute 96-hour LC50 of 10.8 mg/L and a Chronic Value of 1.6 mg/L.
F020 260617
EOR
F002 520
F010 4.1
F004 2
F005 RE
F006 Cash G and Nabholz V (1999). ECOSAR Classes for Microsoft Windows, ECOWIN
*    v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment
*    Division. Washington, DC, USA.
F007 Cash G and Nabholz V (1999). ECOSAR Classes for Microsoft Windows, ECOWIN
*    v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment
*    Division. Washington, DC, USA.
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F020 260619
EOR
F002 520
F010 4.1
F004 2
F005 RL
F006 The value was calculated based on chemical structure as modeled by
* EPIWIN. This robust summary has a reliability rating of 2 because the
* data are calculated and not measured.
F007 The value was calculated based on chemical structure as modeled by
* EPIWIN. This robust summary has a reliability rating of 2 because the
* data are calculated and not measured.
F020 260618
EOR
F002 520
F010 4.1
F004 2
F005 TC
F006 Log Kow (octanol/water partition coefficient) values and a chemical
* structure are needed to calculate aquatic toxicity using the ECOSAR
* model. The Kow calculation is performed by KOWWIN based on an
* atom/fragment contribution method of Meyl
F007 Log Kow (octanol/water partition coefficient) values and a chemical
* structure are needed to calculate aquatic toxicity using the ECOSAR
* model. The Kow calculation is performed by KOWWIN based on an
* atom/fragment contribution method of Meylan and Howard (1), which is a
* subroutine in the EPISuite computer model (2).
**
**
** 1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for
* estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.
**
** 2. EPI SuiteTM (2000). Estimation Program Interface Suite, version 3.12.
* Syracuse Research Corporation, Syracuse, NY, USA.
F020 260616
EOR
F002 520
F010 4.1
F004 2
F005 TS
F006 Analogue substance CAS No. 142-96-1; n-butyl ether
F007 Analogue substance CAS No. 142-96-1; n-butyl ether
F020 260615
EOR
F002 520
F010 4.1
F004 3
F005 RE
F006 Chemicals Inspection and Testing Institute (CITI) (1992). Biodegradation
* and bioaccumulation data of existing chemicals based on the CSCL Japan.
* CITI (ed.). Chemical Products Safety Division, Basic Industries Bureau,
* Ministry of Internatio
F007 Chemicals Inspection and Testing Institute (CITI) (1992). Biodegradation
* and bioaccumulation data of existing chemicals based on the CSCL Japan.
* CITI (ed.). Chemical Products Safety Division, Basic Industries Bureau,
* Ministry of International Trade and Industry, Japan. Japan Chemical
* Industry Ecology-Toxicology and Information Center.

F020 260622
EOR
F002 520
F010 4.1
F004 3
F005 RL
F006 Although a standard method was not followed, the testing procedures
* followed generally accepted fish acute toxicity guideline methods and
* although there was limited information on the specifics of the study,
* there was sufficient information
F007 Although a standard method was not followed, the testing procedures
* followed generally accepted fish acute toxicity guideline methods and
* although there was limited information on the specifics of the study,
* there was sufficient information on testing method and conditions in
* general to rate this study a 2.
F020 260623
EOR
F002 520
F010 4.1
F004 3
F005 TC
F006 Fish supplier was Nakashima fish farm, Kumamoto, Japan. Upon arrival,
* fish were placed in an acclimation tank with a flow-through water system
* for 3 to 5 weeks after external disinfection. The external disinfection
* was carried out under s
F007 Fish supplier was Nakashima fish farm, Kumamoto, Japan. Upon arrival,
* fish were placed in an acclimation tank with a flow-through water system
* for 3 to 5 weeks after external disinfection. The external disinfection
* was carried out under static conditions for about 24-hours in an acqueous
* solution containing 20 mg/l of Elbarju (Ueno Pharm. Co.) and 7 g/l sodium
* chloride.
**
** Test fish were then placed in an acclimation tank with a flow-through
* system at 25°±2°C for about 28 days.
**
** Dilution water for the test and culture was provided by a well of the
* Kurume Research Laboratories. Water temperature, pH, and dissolved
* oxygen were continuously monitored in the laboratory. Total hardness,
* evaporated residue, chemical oxygen demand, chloride ion, and other
* harmful substances were also monitored. The quality of the dilution
* water was confirmed to meet the standards of the Ministry of Health and
* Welfare in total hardness and evaporated residue. The other analyzed
* items met the water quality standards for fisheries.
**
** Test tanks were round glass vessels with 4 liters of test water per
* level. The test was conducted at 25°±2°C. Ten fish were tested at each
* level for 48 hours under semi-static conditions (renewal of test water
* every 8 to 16 hours).
**
** Test concentrations (levels) were not reported.
**
** The 48-hour LC50 value was estimated by either the Doudoroff Method or
* the Probit Method.
F020 260621
EOR
F002 520
F010 4.1

F004 3
F005 TS
F006 Analogue substance CAS No. 142-96-1; n-butyl ether
F007 Analogue substance CAS No. 142-96-1; n-butyl ether
F020 260620
EOR
F002 520
F010 4.2
F004 1
F005 CL
F006 Based on the calculated Kow value of 2.87, sec-Butyl Ether is expected to
* have an acute 48-hour EC50 of 16.7 mg/L and a Chronic Value of 1.3 mg/L.
F007 Based on the calculated Kow value of 2.87, sec-Butyl Ether is expected to
* have an acute 48-hour EC50 of 16.7 mg/L and a Chronic Value of 1.3 mg/L.
F020 260625
EOR
F002 520
F010 4.2
F004 1
F005 RE
F006 Cash G and Nabholz V (1999). ECOSAR Classes for Microsoft Windows, ECOWIN
* v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment
* Division. Washington, DC, USA.
F007 Cash G and Nabholz V (1999). ECOSAR Classes for Microsoft Windows, ECOWIN
* v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment
* Division. Washington, DC, USA.
F020 260627
EOR
F002 520
F010 4.2
F004 1
F005 RL
F006 The value was calculated based on chemical structure as modeled by
* EPIWIN. This robust summary has a reliability rating of 2 because the
* data are calculated and not measured.
F007 The value was calculated based on chemical structure as modeled by
* EPIWIN. This robust summary has a reliability rating of 2 because the
* data are calculated and not measured.
F020 260626
EOR
F002 520
F010 4.2
F004 1
F005 TC
F006 Log Kow (octanol/water partition coefficient) values and a chemical
* structure are needed to calculate aquatic toxicity using the ECOSAR
* model. The Kow calculation is performed by KOWWIN based on an
* atom/fragment contribution method of Meyl
F007 Log Kow (octanol/water partition coefficient) values and a chemical
* structure are needed to calculate aquatic toxicity using the ECOSAR
* model. The Kow calculation is performed by KOWWIN based on an
* atom/fragment contribution method of Meylan and Howard (1), which is a
* subroutine in the EPISuite computer model (2).
**
**
** 1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for
* estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.

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**
**   2.  EPI SuiteTM (2000). Estimation Program Interface Suite, version 3.12.
*    Syracuse Research Corporation, Syracuse, NY, USA.
F020 260624
EOR
F002 520
F010 4.2
F004 1
F005 TS
F006 CAS No. 6863-58-7; sec-butyl ether
F007 CAS No. 6863-58-7; sec-butyl ether
F020 260555
EOR
F002 520
F010 4.2
F004 2
F005 CL
F006 Based on the calculated Kow value of 3.01, n-Butyl Ether is expected to
*    have an acute 48-hour EC50 of 12.5 mg/L and a Chronic Value of 1.0 mg/L.
F007 Based on the calculated Kow value of 3.01, n-Butyl Ether is expected to
*    have an acute 48-hour EC50 of 12.5 mg/L and a Chronic Value of 1.0 mg/L.
F020 260630
EOR
F002 520
F010 4.2
F004 2
F005 RE
F006 Cash G and Nabholz V (1999). ECOSAR Classes for Microsoft Windows, ECOWIN
*    v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment
*    Division. Washington, DC, USA.
F007 Cash G and Nabholz V (1999). ECOSAR Classes for Microsoft Windows, ECOWIN
*    v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment
*    Division. Washington, DC, USA.
F020 260632
EOR
F002 520
F010 4.2
F004 2
F005 RL
F006 The value was calculated based on chemical structure as modeled by
*    EPIWIN.  This robust summary has a reliability rating of 2 because the
*    data are calculated and not measured.
F007 The value was calculated based on chemical structure as modeled by
*    EPIWIN.  This robust summary has a reliability rating of 2 because the
*    data are calculated and not measured.
F020 260631
EOR
F002 520
F010 4.2
F004 2
F005 TC
F006 Log Kow (octanol/water partition coefficient) values and a chemical
*    structure are needed to calculate aquatic toxicity using the ECOSAR
*    model.  The Kow calculation is performed by KOWWIN based on an
*    atom/fragment contribution method of Meyl
F007 Log Kow (octanol/water partition coefficient) values and a chemical
*    structure are needed to calculate aquatic toxicity using the ECOSAR
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*    model.  The Kow calculation is performed by KOWWIN based on an
*    atom/fragment contribution method of Meylan and Howard (1), which is a
*    subroutine in the EPISuite computer model (2).
**
**
**   1.  Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for
*    estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.
**
**   2.  EPI SuiteTM (2000). Estimation Program Interface Suite, version 3.12.
*    Syracuse Research Corporation, Syracuse, NY, USA.
F020 260629
EOR
F002 520
F010 4.2
F004 2
F005 TS
F006 Analogue substance CAS No. 142-96-1; n-butyl ether
F007 Analogue substance CAS No. 142-96-1; n-butyl ether
F020 260628
EOR
F002 520
F010 4.3
F004 1
F005 CL
F006 Based on the calculated Kow value of 2.87, sec-Butyl Ether is expected to
*    have an acute 96-hour EC50 of 11.0 mg/L and a Chronic Value of 1.8 mg/L.
F007 Based on the calculated Kow value of 2.87, sec-Butyl Ether is expected to
*    have an acute 96-hour EC50 of 11.0 mg/L and a Chronic Value of 1.8 mg/L.
F020 260639
EOR
F002 520
F010 4.3
F004 1
F005 RE
F006 Cash G and Nabholz V (1999). ECOSAR Classes for Microsoft Windows, ECOWIN
*    v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment
*    Division. Washington, DC, USA.
F007 Cash G and Nabholz V (1999). ECOSAR Classes for Microsoft Windows, ECOWIN
*    v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment
*    Division. Washington, DC, USA.
F020 260641
EOR
F002 520
F010 4.3
F004 1
F005 RL
F006 The value was calculated based on chemical structure as modeled by
*    EPIWIN.  This robust summary has a reliability rating of 2 because the
*    data are calculated and not measured.
F007 The value was calculated based on chemical structure as modeled by
*    EPIWIN.  This robust summary has a reliability rating of 2 because the
*    data are calculated and not measured.
F020 260640
EOR
F002 520
F010 4.3
F004 1
```

F005 TC
F006 Log Kow (octanol/water partition coefficient) values and a chemical
*   structure are needed to calculate aquatic toxicity using the ECOSAR
*   model. The Kow calculation is performed by KOWWIN based on an
*   atom/fragment contribution method of Meyl
F007 Log Kow (octanol/water partition coefficient) values and a chemical
*   structure are needed to calculate aquatic toxicity using the ECOSAR
*   model. The Kow calculation is performed by KOWWIN based on an
*   atom/fragment contribution method of Meylan and Howard (1), which is a
*   subroutine in the EPISuite computer model (2).
**
**
**   1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for
*   estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.
**
**   2. EPI SuiteTM (2000). Estimation Program Interface Suite, version 3.12.
*   Syracuse Research Corporation, Syracuse, NY, USA.
F020 260638
EOR
F002 520
F010 4.3
F004 1
F005 TS
F006 CAS No. 6863-58-7; sec-butyl ether
F007 CAS No. 6863-58-7; sec-butyl ether
F020 260556
EOR
F002 520
F010 4.3
F004 2
F005 CL
F006 Based on the calculated Kow value of 3.01, n-Butyl Ether is expected to
*   have an acute 96-hour EC50 of 8.3 mg/L and a Chronic Value of 1.5 mg/L.
F007 Based on the calculated Kow value of 3.01, n-Butyl Ether is expected to
*   have an acute 96-hour EC50 of 8.3 mg/L and a Chronic Value of 1.5 mg/L.
F020 260644
EOR
F002 520
F010 4.3
F004 2
F005 RE
F006 Cash G and Nabholz V (1999). ECOSAR Classes for Microsoft Windows, ECOWIN
*   v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment
*   Division. Washington, DC, USA.
F007 Cash G and Nabholz V (1999). ECOSAR Classes for Microsoft Windows, ECOWIN
*   v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment
*   Division. Washington, DC, USA.
F020 260646
EOR
F002 520
F010 4.3
F004 2
F005 RL
F006 The value was calculated based on chemical structure as modeled by
*   EPIWIN. This robust summary has a reliability rating of 2 because the
*   data are calculated and not measured.
F007 The value was calculated based on chemical structure as modeled by

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*    EPIWIN.  This robust summary has a reliability rating of 2 because the
*    data are calculated and not measured.
F020 260645
EOR
F002 520
F010 4.3
F004 2
F005 TC
F006 Log Kow (octanol/water partition coefficient) values and a chemical
*    structure are needed to calculate aquatic toxicity using the ECOSAR
*    model.  The Kow calculation is performed by KOWWIN based on an
*    atom/fragment contribution method of Meyl
F007 Log Kow (octanol/water partition coefficient) values and a chemical
*    structure are needed to calculate aquatic toxicity using the ECOSAR
*    model.  The Kow calculation is performed by KOWWIN based on an
*    atom/fragment contribution method of Meylan and Howard (1), which is a
*    subroutine in the EPISuite computer model (2).
**
**
**   1.  Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for
*    estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.
**
**   2.  EPI SuiteTM (2000). Estimation Program Interface Suite, version 3.12.
*    Syracuse Research Corporation, Syracuse, NY, USA.
F020 260643
EOR
F002 520
F010 4.3
F004 2
F005 TS
F006 Analogue substance CAS No. 142-96-1; n-butyl ether
F007 Analogue substance CAS No. 142-96-1; n-butyl ether
F020 260642
EOR
F002 520
F010 4.5.1
F004 1
F005 CL
F006 Based on the calculated Kow value of 2.87, sec-Butyl Ether is expected to
*    have an acute 96-hour LC50 of 14.7 mg/L and a Chronic Value of 2.2 mg/L
F007 Based on the calculated Kow value of 2.87, sec-Butyl Ether is expected to
*    have an acute 96-hour LC50 of 14.7 mg/L and a Chronic Value of 2.2 mg/L
F020 260649
EOR
F002 520
F010 4.5.1
F004 1
F005 RE
F006 Cash G and Nabholz V (1999). ECOSAR Classes for Microsoft Windows, ECOWIN
*    v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment
*    Division. Washington, DC, USA.
F007 Cash G and Nabholz V (1999). ECOSAR Classes for Microsoft Windows, ECOWIN
*    v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment
*    Division. Washington, DC, USA.
F020 260651
EOR
F002 520
```

F010 4.5.1
F004 1
F005 RL
F006 The value was calculated based on chemical structure as modeled by
*   EPIWIN. This robust summary has a reliability rating of 2 because the
*   data are calculated and not measured.
F007 The value was calculated based on chemical structure as modeled by
*   EPIWIN. This robust summary has a reliability rating of 2 because the
*   data are calculated and not measured.
F020 260650
EOR
F002 520
F010 4.5.1
F004 1
F005 TC
F006 Log Kow (octanol/water partition coefficient) values and a chemical
*   structure are needed to calculate aquatic toxicity using the ECOSAR
*   model. The Kow calculation is performed by KOWWIN based on an
*   atom/fragment contribution method of Meyl
F007 Log Kow (octanol/water partition coefficient) values and a chemical
*   structure are needed to calculate aquatic toxicity using the ECOSAR
*   model. The Kow calculation is performed by KOWWIN based on an
*   atom/fragment contribution method of Meylan and Howard (1), which is a
*   subroutine in the EPISuite computer model (2).
**
**
**   1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for
*   estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.
**
**   2. EPI SuiteTM (2000). Estimation Program Interface Suite, version 3.12.
*   Syracuse Research Corporation, Syracuse, NY, USA.
F020 260648
EOR
F002 520
F010 4.5.1
F004 1
F005 TS
F006 CAS No. 6863-58-7; sec-butyl ether
F007 CAS No. 6863-58-7; sec-butyl ether
F020 260647
EOR
F002 520
F010 4.5.1
F004 2
F005 CL
F006 Based on the calculated Kow value of 3.01, n-Butyl Ether is expected to
*   have an acute 96-hour LC50 of 10.8 mg/L and a Chronic Value of 1.6 mg/L.
F007 Based on the calculated Kow value of 3.01, n-Butyl Ether is expected to
*   have an acute 96-hour LC50 of 10.8 mg/L and a Chronic Value of 1.6 mg/L.
F020 260654
EOR
F002 520
F010 4.5.1
F004 2
F005 RE
F006 Cash G and Nabholz V (1999). ECOSAR Classes for Microsoft Windows, ECOWIN
*   v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment

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*    Division. Washington, DC, USA.
F007 Cash G and Nabholz V (1999). ECOSAR Classes for Microsoft Windows, ECOWIN
*    v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment
*    Division. Washington, DC, USA.
F020 260656
EOR
F002 520
F010 4.5.1
F004 2
F005 RL
F006 The value was calculated based on chemical structure as modeled by
*    EPIWIN.  This robust summary has a reliability rating of 2 because the
*    data are calculated and not measured.
F007 The value was calculated based on chemical structure as modeled by
*    EPIWIN.  This robust summary has a reliability rating of 2 because the
*    data are calculated and not measured.
F020 260655
EOR
F002 520
F010 4.5.1
F004 2
F005 TC
F006 Log Kow (octanol/water partition coefficient) values and a chemical
*    structure are needed to calculate aquatic toxicity using the ECOSAR
*    model.  The Kow calculation is performed by KOWWIN based on an
*    atom/fragment contribution method of Meyl
F007 Log Kow (octanol/water partition coefficient) values and a chemical
*    structure are needed to calculate aquatic toxicity using the ECOSAR
*    model.  The Kow calculation is performed by KOWWIN based on an
*    atom/fragment contribution method of Meylan and Howard (1), which is a
*    subroutine in the EPISuite computer model (2).
F020 260653
EOR
F002 520
F010 4.5.1
F004 2
F005 TS
F006 Analogue substance CAS No. 142-96-1; n-butyl ether
F007 Analogue substance CAS No. 142-96-1; n-butyl ether
F020 260652
EOR
F002 520
F010 4.5.2
F004 1
F005 CL
F006 Based on the calculated Kow value of 2.87, sec-Butyl Ether is expected to
*    have an acute 48-hour EC50 of 16.7 mg/L and a Chronic Value of 1.3 mg/L.
F007 Based on the calculated Kow value of 2.87, sec-Butyl Ether is expected to
*    have an acute 48-hour EC50 of 16.7 mg/L and a Chronic Value of 1.3 mg/L.
F020 260659
EOR
F002 520
F010 4.5.2
F004 1
F005 RE
F006 Cash G and Nabholz V (1999). ECOSAR Classes for Microsoft Windows, ECOWIN
*    v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment
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*    Division. Washington, DC, USA.
F007 Cash G and Nabholz V (1999). ECOSAR Classes for Microsoft Windows, ECOWIN
*    v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment
*    Division. Washington, DC, USA.
F020 260661
EOR
F002 520
F010 4.5.2
F004 1
F005 RL
F006 The value was calculated based on chemical structure as modeled by
*    EPIWIN.  This robust summary has a reliability rating of 2 because the
*    data are calculated and not measured.
F007 The value was calculated based on chemical structure as modeled by
*    EPIWIN.  This robust summary has a reliability rating of 2 because the
*    data are calculated and not measured.
F020 260660
EOR
F002 520
F010 4.5.2
F004 1
F005 TC
F006 Log Kow (octanol/water partition coefficient) values and a chemical
*    structure are needed to calculate aquatic toxicity using the ECOSAR
*    model.  The Kow calculation is performed by KOWWIN based on an
*    atom/fragment contribution method of Meyl
F007 Log Kow (octanol/water partition coefficient) values and a chemical
*    structure are needed to calculate aquatic toxicity using the ECOSAR
*    model.  The Kow calculation is performed by KOWWIN based on an
*    atom/fragment contribution method of Meylan and Howard (1), which is a
*    subroutine in the EPISuite computer model (2).
**
**
**   1.  Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for
*    estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.
**
**   2.  EPI SuiteTM (2000). Estimation Program Interface Suite, version 3.12.
*    Syracuse Research Corporation, Syracuse, NY, USA.
F020 260658
EOR
F002 520
F010 4.5.2
F004 1
F005 TS
F006 CAS No. 6863-58-7; sec-butyl ether
F007 CAS No. 6863-58-7; sec-butyl ether
F020 260657
EOR
F002 520
F010 4.5.2
F004 2
F005 CL
F006 Based on the calculated Kow value of 3.01, n-Butyl Ether is expected to
*    have an acute 48-hour EC50 of 12.5 mg/L and a Chronic Value of 1.0 mg/L.
F007 Based on the calculated Kow value of 3.01, n-Butyl Ether is expected to
*    have an acute 48-hour EC50 of 12.5 mg/L and a Chronic Value of 1.0 mg/L.
F020 260667
```

EOR
F002 520
F010 4.5.2
F004 2
F005 RE
F006 Cash G and Nabholz V (1999). ECOSAR Classes for Microsoft Windows, ECOWIN
* v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment
* Division. Washington, DC, USA.
F007 Cash G and Nabholz V (1999). ECOSAR Classes for Microsoft Windows, ECOWIN
* v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment
* Division. Washington, DC, USA.
F020 260669
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F002 520
F010 4.5.2
F004 2
F005 RL
F006 The value was calculated based on chemical structure as modeled by
* EPIWIN. This robust summary has a reliability rating of 2 because the
* data are calculated and not measured.
F007 The value was calculated based on chemical structure as modeled by
* EPIWIN. This robust summary has a reliability rating of 2 because the
* data are calculated and not measured.
F020 260668
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F005 TC
F006 Log Kow (octanol/water partition coefficient) values and a chemical
* structure are needed to calculate aquatic toxicity using the ECOSAR
* model. The Kow calculation is performed by KOWWIN based on an
* atom/fragment contribution method of Meyl
F007 Log Kow (octanol/water partition coefficient) values and a chemical
* structure are needed to calculate aquatic toxicity using the ECOSAR
* model. The Kow calculation is performed by KOWWIN based on an
* atom/fragment contribution method of Meylan and Howard (1), which is a
* subroutine in the EPISuite computer model (2).
**
**
** 1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for
* estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.
**
** 2. EPI SuiteTM (2000). Estimation Program Interface Suite, version 3.12.
* Syracuse Research Corporation, Syracuse, NY, USA.
F020 260666
EOR
F002 520
F010 4.5.2
F004 2
F005 TS
F006 Analogue substance CAS No. 142-96-1; n-butyl ether
F007 Analogue substance CAS No. 142-96-1; n-butyl ether
F020 260665
EOB
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B005 SUBST_MASTER_TAB
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B006 SUBST_IDENT_TAB
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F003 Y27-006
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F003 Y27-002
F004 203-560-6
F005 3
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F001 108-20-3
F002 Y28-002
F003 Y27-030
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F005 4
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F001 108-20-3
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F003 Y27-003
F004 C6H14O
F005 102
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B003 DS_ADMIN_TAB
F002 455
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F102 A35-02
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B004 COMPANY_TAB
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F004 1545 Route 22 East
F005 Annadale, New Jersey
F006 08801-3059
F008 A31-024
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B052 DS_COMPONENT_JOIN_TAB
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F005 2
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F001 455
F002 0
F003 2.3
F004 2
F005 2
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F004 2
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F007 27-10-2005
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F003 3.5
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F005 12
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B053 DS_REC_MARK_TAB
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F002 2.6.1
F003 2
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F001 455

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B051 DS_COMPONENT_TAB
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F008 HPV
F009 A35-02
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F003 108-20-3
F012 N
F010 10-02-2000
F011 10-02-2000
F004 101
F005 10-02-2000
F006 101
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F007 10-02-2000
F009 A35-02
EOB
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B101 GI_GENERAL_INFORM_TAB
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F004 CLGETTS
F010 A04-04
F011 A19-02
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B102 GI_SYNONYM_TAB
F001 455
F002 1
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F004 CLGETTS
F007 2,2'-oxybis-propane
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F002 2
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F004 CLGETTS
F007 IPE
EOR
F001 455
F002 3
F003 27-10-2005
F004 CLGETTS
F007 2-isopropoxypropane
EOR
F001 455
F002 4
F003 27-10-2005
F004 CLGETTS
F007 IPE; Diisopropylether; DIPE; 2-Isopropoxy propane
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F002 5
F003 27-10-2005
F004 CLGETTS
F007 Diisopropyl Ether
EOR
F001 455
F002 6
F003 27-10-2005
F004 CLGETTS
F007 Isopropyl Ether
EOR
F001 455
F002 8
F003 27-10-2005
F004 CLGETTS
F007 2-Isopropoxy Propane
EOR
F001 455

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F004 CLGETTS
F007 propane, 2,2'-oxybis-
EOR
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F003 27-10-2005
F004 CLGETTS
F007 2,2'-oxybispropane
EOR
F001 455
F002 11
F003 27-10-2005
F004 CLGETTS
F007 Isopropylether
EOR
F001 455
F002 12
F003 27-10-2005
F004 CLGETTS
F007 Dipropyloxid
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F001 455
F002 14
F003 27-10-2005
F004 CLGETTS
F007 2-Isopropoxypropan
EOB
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B201 PC_MELTING_TAB
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F016 1
F007 A02-03
F008 -86.8
F012 P01-03: not specified
F014 A03-02
F020 A01-03: Diisopropyl Ether (CAS # 108-20-3)
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B202 PC_BOILING_TAB
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F004 CLGETTS
F016 A36-003
F017 1
F007 A02-03
F008 68.5
F010 1013
F011 P02-01
F013 P03-03: not specified
F015 A03-02

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F018 A01-03: Diisopropylether
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B203 PC_DENSITY_TAB
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F008 A02-03
F009 .7241
F011 P18-01
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F015 A03-02
F018 A01-03:  Diisopropyl Ether (CAS # 108-20-3)
EOB
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B204 PC_VAPOUR_TAB
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F004 CLGETTS
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F016 1
F007 A02-03
F008 198.65
F010 P02-01
F011 25
F014 A03-02
F018 A01-03:  Diisopropyl Ether (CAS # 108-20-3)
EOB
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B205 PC_PARTITION_TAB
F001 455
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F004 CLGETTS
F014 A36-003
F015 1
F007 A02-03
F008 1.52
F010 25
F011 P07-05
F013 A03-02
F016 A01-03: Diisopropylether
F020 C15-001
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F001 455
F002 3
F003 12-12-2005
F004 CLGETTS
F014 A36-002
F015 2
F007 A02-03
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F008 2.4
F011 P07-04:  Indirect method by reverse-phase HPLC
F013 A03-01
F016 A01-03:  diisopropyl ether (CAS No. 108-20-3)
F020 C15-001
F019 6.7
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B206 PC_WATER_SOL_TAB
F001 455
F002 2
F003 07-12-2005
F004 CLGETTS
F023 A36-003
F024 1
F007 A02-03
F008 P08-02
F009 8800
F011 20
F022 A03-02
F025 A01-03:  Diisopropyl Ether (CAS # 108-20-3)
F030 C14-001
EOB
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B301 EN_PHOTODEGRADATION_TAB
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F004 CLGETTS
F045 A36-003
F046 1
F007 A01-03:  Diisopropyl Ether (CAS # 108-20-3)
F008 F01-01
F009 F02-05:  Calculated values using AOPWIN version 1.89, a subroutine of the
*    computer program EPIWIN version 3.12
F023 25
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F035 1500000
F036 F07-02
F044 A02-03
F037 .00000000002434
F038 A02-03
F040 50
F041 5.3
F042 F05-02
EOR
F001 455
F002 3
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F004 CLGETTS
F045 A36-003
F046 2
F007 A01-03:  Diisopropyl Ether (CAS # 108-20-3)
EOB
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B302 EN_STABILITY_IN_WATER_TAB
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F041 1
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F008 F08-01
F009 F09-03:  Technical discussion
F039 A03-02
EOB
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B305 EN_TRANSPORT_TAB
F001 455
F002 2
F003 07-12-2005
F004 CLGETTS
F011 A36-003
F012 1
F008 F22-01:  air - biota - sediment(s) - soil - water
F009 F21-01:  Calculation according Mackay, Level I
EOR
F001 455
F002 3
F003 01-11-2005
F004 CLGETTS
F011 A36-003
F012 2
F007 F20-07
F008 F22-01
F009 F21-01:  Level III simulation using the Mackay Multimedia Environmental
*    Model (Mackay, 2001)
EOB
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B308 EN_BIODEGRADATION_TAB
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F004 CLGETTS
F047 A36-002
F048 1
F007 A01-03:  Diisopropyl Ether (CAS No. 108-20-3)
F008 F25-01
F009 F26-18
F010 1982
F011 F27-0139
F020 F30-02:  not readily biodegradable
F046 A03-01
F052 28
F053 F05-01
EOR
F001 455
F002 3
F003 07-02-2006
F004 CLGETTS
F047 A36-003
F048 2
F007 A01-03:  diisopropyl ether (CAS No. 108-20-3)
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F009 F26-25: American Public Health Association; No. 219 5-Day BOD; Standard
*   Dilution Method
F010 1971
F011 F27-0166: sanitary waste treatment plant effluent
F046 A03-01
F052 5
F053 F05-01
EOR
F001 455
F002 4
F003 07-02-2006
F004 CLGETTS
F047 A36-003
F048 3
F007 A01-03:   diisopropyl ether (CAS No. 108-20-3)
F008 F25-01
F009 F26-25: (comparison study of three aerobic biodegradation methods)
F010 1997
F011 F27-0137
F046 A03-01
EOR
F001 455
F002 5
F003 07-02-2006
F004 CLGETTS
F047 A36-003
F048 4
F007 A01-03: diisopropyl ether (CAS No. 108-20-3)
F008 F25-01
F009 F26-25: (continuous-flow bioreactors)
F010 2001
F011 F27-0166: Mixture (see remarks)
F046 A03-01
F052 600
F053 F05-01
EOR
F001 455
F002 6
F003 07-02-2006
F004 CLGETTS
F047 A36-003
F048 5
F007 A01-03: diisopropyl ether (CAS No. 108-20-3)
F009 F26-25: (soil/water microcosm)
F010 1999
F011 F27-0166: soil and groundwater from a site previously exposed to methyl
*   tert-butyl ether
F046 A03-01
F052 1
F053 F05-05
EOR
F001 455
F002 7
F003 07-02-2006
F004 CLGETTS
F047 A36-003
F048 6

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F007 A01-03:  diisopropyl ether (CAS No. 108-20-3)
F008 F25-02
F009 F26-25: (closed serum bottle test)
F010 1993
F011 F27-0166:  sediment and groundwater from an anoxic aquifer polluted by
*    municipal landfill leachate
F046 A03-01
F052 252
F053 F05-01
EOR
F001 455
F002 8
F003 24-02-2006
F004 CLGETTS
F047 A36-003
F048 7
F007 A01-03:  diisopropyl ether (CAS No. 108-20-3)
F008 F25-02
F009 F26-25:  unknown
F010 1994
F011 F27-0166:  Sediment and surface or groundwater
F046 A03-01
EOR
F001 455
F002 9
F003 07-02-2006
F004 CLGETTS
F047 A36-003
F048 8
F007 A01-03:  diisopropyl ether (CAS No. 108-20-3)
F008 F25-01
F009 F26-25:  (sealed flasks, shaken)
F010 2000
F011 F27-0166:  Gordonia terrae strain IFP 2001 (CNCM Registration No. CTP
*    1-1889); isolated from activated sludge taken at an urban waste water
*    treatment plant
F046 A03-01
F052 24
F053 F05-02
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B310 EN_BIOACCUMULATION_TAB
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F021 A36-003
F022 1
F007 A01-03:  Diisopropyl Ether (CAS # 108-20-3)
F008 E02-0161:  see remark
F009 F34-06:  calculation
F015 25
F016 A02-03
F017 2.95
F020 A03-01
EOR
F001 455
```

F002 2
F003 12-12-2005
F004 CLGETTS
F021 A36-003
F022 2
F007 A01-03: Diisopropyl Ether (CAS No. 108-20-3)
F008 E02-0161: see remark
F009 F34-06: calculation
F015 25
F016 A02-03
F017 14.06
F020 A03-01
EOB
C
B311 EN_OTHER_TAB
F001 455
F002 1
F003 07-02-2006
F004 CLGETTS
F010 1
F009 Biodegradation of diisopropyl ether
EOR
F001 455
F002 2
F003 27-02-2006
F004 CLGETTS
F010 2
F009 Biodegradation of diisopropyl ether under aerobic and anaerobic
*   conditions - summary
EOB
C
B401 EC_FISHTOX_TAB
F001 455
F002 1
F003 01-11-2005
F004 CLGETTS
F033 A36-003
F034 1
F007 A01-03: Diisopropyl Ether (CAS No. 108-20-3)
F008 E01-02
F009 E02-0119
F010 E03-05: Flow-through Fish Acute Toxicity Test
F011 1983
F012 96
F013 E04-02
F014 E05-02
F021 A02-03
F022 91.7
F031 A03-03
F032 A03-02
EOR
F001 455
F002 2
F003 28-10-2005
F004 CLGETTS
F033 A36-003
F034 2

F007 A01-03: Diisopropyl Ether (CAS No. 108-20-3)
F009 E02-0161: Fish
F010 E03-05: ECOSAR version 0.99h, US EPA
F012 96
F013 E04-02
F014 E05-02
F021 A02-03
F022 214.1
EOR
F001 455
F002 3
F003 12-12-2005
F004 CLGETTS
F033 A36-002
F034 3
F007 A01-03: Diisopropyl Ether (CAS No. 108-20-3)
F008 E01-02
F009 E02-0119
F010 E03-05: Flow-through Fish Acute Toxicity Test
F011 1983
F012 96
F013 E04-02
F014 E05-02
F021 A02-03
F022 786
F027 EC50
F028 A02-03
F029 476
F031 A03-03
F032 A03-02
EOR
F001 455
F002 4
F003 12-12-2005
F004 CLGETTS
F033 A36-002
F034 4
F007 A01-03: Diisopropyl Ether (CAS No. 108-20-3)
F008 E01-02
F009 E02-0119
F010 E03-05: Flow-through Fish Acute Toxicity Test (ASTM, 1980)
F011 1985
F012 96
F013 E04-02
F014 E05-02
F021 A02-03
F022 900
F031 A03-03
F032 A03-02
EOR
F001 455
F002 5
F003 12-12-2005
F004 CLGETTS
F033 A36-004
F034 5
F007 A01-03: Diisopropyl Ether (CAS No. 108-20-3)

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F008 E01-05
F009 E02-0015
F010 E03-05: static acute fish toxicity test (APHA, 1971)
F012 24
F013 E04-02
F014 E05-02
F021 A02-03
F022 380
F031 A03-03
F032 A03-02
EOR
F001 455
F002 6
F003 12-12-2005
F004 CLGETTS
F033 A36-004
F034 6
F007 A01-03: Diisopropyl Ether (CAS No. 108-20-3)
F008 E01-05
F009 E02-0070
F010 E03-05: static acute fish toxicity test
F012 96
F013 E04-02
F014 E05-02
F022 7000
F031 A03-01
F032 A03-01
EOR
F001 455
F002 7
F003 12-12-2005
F004 CLGETTS
F033 A36-004
F034 7
F007 A01-03: Diisopropyl Ether (CAS No. 108-20-3)
F008 E01-05
F009 E02-0082
F010 E03-05: static acute fish toxicity test
F012 96
F013 E04-02
F014 E05-02
F022 6600
F031 A03-01
F032 A03-01
EOB
C
B402 EC_DAPHNIATOX_TAB
F001 455
F002 1
F003 07-12-2005
F004 CLGETTS
F032 A36-003
F033 1
F007 A01-03:  Diisopropyl Ether (CAS No. 108-20-3)
F008 E06-0010
F009 E07-04: U.S. Environmental Protection Agency, Methods for acute toxicity
*    testing with fish, macro-invertebrates and amphibians (EPA-660/3-75-009)
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F010 1975
F011 48
F012 E04-02
F013 E05-02
F020 A02-03
F021 190
F030 A03-01
F031 A03-01
EOR
F001 455
F002 2
F003 28-10-2005
F004 CLGETTS
F032 A36-003
F033 2
F007 A01-03: Diisopropyl Ether (CAS No. 108-20-3)
F008 E06-0034: Daphnia
F009 E07-04: ECOSAR version 0.99h, US EPA
F011 48
F012 E04-02
F013 E05-02
F020 A02-03
F021 221.9
EOB
C
B403 EC_ALGAETOX_TAB
F001 455
F002 2
F003 28-10-2005
F004 CLGETTS
F036 A36-003
F037 1
F007 A01-03: Diisopropyl Ether (CAS No. 108-20-3)
F008 E08-0063: Green Alga
F009 E09-04: ECOSAR version 0.99h, US EPA
F012 96
F013 E04-02
F014 E05-02
F027 A02-03
F028 134.9
F030 ChV
F031 A02-03
F032 10.2
EOR
F001 455
F002 3
F003 12-12-2005
F004 CLGETTS
F036 A36-004
F037 2
F007 A01-03: Diisopropyl Ether (CAS No. 108-20-3)
F008 E08-0056
F009 E09-04: algae growth inhibition
F010 1983
F011 E10-01
F012 96
F013 E04-02

F014 E05-02
F027 A02-05
F028 1000
F034 A03-01
F035 A03-02
EOB
C
B501 TO_ACUTE_ORAL_TAB
F001 455
F002 5
F003 01-11-2005
F004 CLGETTS
F017 A36-003
F018 1
F007 A01-03: Diisopropyl ether (CAS No. 108-20-3)
F008 T01-03
F009 T02-24
F010 T03-03: Similar to OECD 401
F016 A03-01
F019 T24-03
F021 T52-003: None; administered undiluted
F022 T23-42
EOR
F001 455
F002 6
F003 01-11-2005
F004 CLGETTS
F017 A36-003
F018 2
F007 A01-03: Diisopropyl ether (CAS No. 108-20-3)
F009 T02-23
F010 T03-03: Similar to OECD 401
F016 A03-01
F019 T24-04
F020 6
F021 T52-003: none reported
F022 T23-31
F023 8.2, 7.2, 6.0, 5.2, 3.3, 1.62 g/kg
EOB
C
B502 TO_ACUTE_INHAL_TAB
F001 455
F002 2
F003 01-11-2005
F004 CLGETTS
F019 A36-003
F020 1
F007 A01-03: Diisopropyl ether (CAS No. 108-20-3)
F009 T02-10
F010 T06-03: not specified
F018 A03-01
F021 T24-04
F023 T52-003: none
F024 T23-48: not specified
F025 0.3%; 1%; 3%; 6% in air
EOR
F001 455

F002 3
F003 01-11-2005
F004 CLGETTS
F019 A36-003
F020 2
F007 A01-03: Diisopropyl ether (CAS No. 108-20-3)
F009 T02-23
F010 T06-03: not specified
F018 A03-01
F021 T24-04
F023 T52-003: none
F024 T23-31
F025 0.3%; 1%; 3%; 6% in air
EOR
F001 455
F002 4
F003 01-11-2005
F004 CLGETTS
F019 A36-003
F020 3
F007 A01-03: Diisopropyl ether (CAS No. 108-20-3)
F009 T02-17
F010 T06-03: not specified
F018 A03-01
F021 T24-01
F023 T52-003: none
F024 T23-48: Macacus rhesus
F025 0.3%; 1%; 3%; 6% in air
EOB
C
B503 TO_ACUTE_DERMAL_TAB
F001 455
F002 2
F003 01-11-2005
F004 CLGETTS
F017 A36-003
F018 1
F007 A01-03: Diisopropyl ether (CAS No. 108-20-3)
F008 T01-03
F009 T02-23
F010 T09-02: Similar to OECD 402
F016 A03-01
F019 T24-04
F021 T52-003: none
F022 T23-31
F023 variable
EOB
C
B507 TO_SENSITIZATION_TAB
F001 455
F002 2
F003 01-11-2005
F004 CLGETTS
F015 A36-003
F016 1
F007 A01-03: Diisopropyl ether (CAS No.108-20-3)
F008 T18-14: In vitro chemical reactivity assay, surrogate for respiratory

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*    sensitization
F009 T02-19:  No animals; in vitro chemical assay
F010 T20-03:  No guideline available
F011 1990
F012 T47-01
F013 T21-02
F014 A03-01
F017 0
F030 T52-003:  None
EOB
C
B508 TO_REPEATED_DOSE_TAB
F001 455
F002 5
F003 01-11-2005
F004 CLGETTS
F030 A36-003
F031 1
F007 A01-03:  Diisopropyl Ether (CAS No. 108-20-3)
F008 T02-24
F009 T23-42
F010 T24-03
F011 T25-08
F012 T26-23
F013 1996
F014 6 hours/day
F015 5 days/week for ~13 weeks
F017 0, 480, 3300, or 7100 ppm
F018 T27-03:  yes (untreated & sham-exposed)
F019 A02-03
F020 480
F022 T28-05
F029 A03-02
F032 C07-002
EOR
F001 455
F002 6
F003 01-11-2005
F004 CLGETTS
F030 A36-003
F031 2
F007 A01-03:  Diisopropyl Ether (CAS No. 108-20-3)
F008 T02-24
F009 T23-42
F010 T24-03
F011 T25-08
F012 T26-16:  USEPA 1984, 40CFR Part 798:6050, 6400, and 6200
F013 1997
F014 6 hours/day
F015 5 days/week for ~13 weeks
F017 0, 450, 3250, or 7060 ppm
F018 T27-03:  yes (sham-exposed)
F029 A03-02
F032 C07-002
EOB
C
B509 TO_GENETIC_IN_VITRO_TAB
```

F001 455
F002 4
F003 10-11-2005
F004 CLGETTS
F016 A36-003
F017 1
F007 A01-03: Diisopropyl ether (CAS No. 108-20-3)
F008 T30-05
F009 T31-18: Similar to OECD Guideline 471
F010 1988
F011 Salmonella typhimurium
F012 T32-03
F013 T33-02
F014 A03-02
F015 Up to 8000 ug/ml in the pre-incubation mix
EOR
F001 455
F002 5
F003 10-11-2005
F004 CLGETTS
F016 A36-003
F017 2
F007 A01-03: Di-isopropyl ether (CAS No. 108-20-3)
F008 T30-15
F009 T31-18: Similar to OECD Guideline 473
F010 1984
F011 Chinese hamster ovary cells
F012 T32-04
F013 T33-02
F014 A03-02
F015 Up to 1200 ug/ml
EOR
F001 455
F002 6
F003 10-11-2005
F004 CLGETTS
F016 A36-003
F017 3
F007 A01-03: Di-isopropyl ether (CAS No. 108-20-3)
F008 T30-07
F009 T31-18: Similar to OECD Guideline 476
F010 1984
F011 Rat liver cells
F012 T32-04
F013 T33-02
F014 A03-02
F015 Up to 1200 ug/ml
EOR
F001 455
F002 7
F003 10-11-2005
F004 CLGETTS
F016 A36-003
F017 4
F007 A01-03: Di-isopropyl ether (CAS No. 108-20-3)
F008 T30-09
F009 T31-18: Similar to OECD Guideline 481

F010 1984
F011 Saccharomyces cerevisiae
F012 T32-03
F013 T33-02
F014 A03-02
F015 Up to 8000 ug/ml in the pre-incubation mix
EOB
C
B513 TO_DEVELOPMENTAL_TAB
F001 455
F002 2
F003 01-11-2005
F004 CLGETTS
F030 A36-003
F007 A01-03: Diisopropyl Ether (CAS No. 108-20-3)
F008 T02-24
F009 T23-42
F010 T24-01
F011 T25-08
F012 T44-06
F013 1996
F014 20 days
F015 6 hr/day
F016 Gestation Days 6-15
F017 0, 430, 3095, or 6745 ppm
F018 T27-03: yes (untreated & sham-exposed)
F029 A03-02
F032 T58-007: NOEL Maternal
F033 A02-03
F034 430
F036 T43-04
F037 T58-007: NOEL Pup
F038 A02-03
F039 430
F041 T43-04
F047 Maternal NOEL: 430 ppm; Pup NOEL: 430 ppm
EOB
C
B514 TO_OTHER_TAB
F001 455
F002 2
F003 01-11-2005
F004 CLGETTS
F008 A36-003
F009 1
F007 T45-12: Sensory Irritation in Humans
EOR
F001 455
F002 3
F003 01-11-2005
F004 CLGETTS
F008 A36-003
F009 2
F007 T45-12: Sensory irritation in humans
EOB
C
B601 TEXT_TAB

F002 455
F010 2.1
F004 2
F005 RE
F006 Lide D, et al. (eds.) (1997-1998). CRC Handbook of Chemistry and Physics.
* 78th Edition. CRC Press, New York, NY, USA.
F007 Lide D, et al. (eds.) (1997-1998). CRC Handbook of Chemistry and Physics.
* 78th Edition. CRC Press, New York, NY, USA.
F020 241178
EOR
F002 455
F010 2.1
F004 2
F005 RL
F006 The CRC Handbook of Chemistry and Physics is a peer reviewed publication.
* This robust summary has a reliability rating of 2 because there is
* insufficient information available on the method and analytical procedure.
F007 The CRC Handbook of Chemistry and Physics is a peer reviewed publication.
* This robust summary has a reliability rating of 2 because there is
* insufficient information available on the method and analytical procedure.
F020 241177
EOR
F002 455
F010 2.1
F004 2
F005 TS
F006 CAS No. 108-20-3; diisopropyl ether; purity is unknown.
F007 CAS No. 108-20-3; diisopropyl ether; purity is unknown.
F020 241176
EOR
F002 455
F010 2.2
F004 2
F005 RE
F006 Lide D, et al. (eds.) (1997-1998). CRC Handbook of Chemistry and Physics.
* 78th Edition. CRC Press, New York, NY, USA.
F007 Lide D, et al. (eds.) (1997-1998). CRC Handbook of Chemistry and Physics.
* 78th Edition. CRC Press, New York, NY, USA.
F020 241181
EOR
F002 455
F010 2.2
F004 2
F005 RL
F006 The CRC Handbook of Chemistry and Physics is a peer reviewed publication.
* This robust summary has a reliability rating of 2 because there is
* insufficient information available on the method and analytical procedure.
F007 The CRC Handbook of Chemistry and Physics is a peer reviewed publication.
* This robust summary has a reliability rating of 2 because there is
* insufficient information available on the method and analytical procedure.
F020 241180
EOR
F002 455
F010 2.2
F004 2
F005 TS
F006 CAS No. 108-20-3; diisopropyl ether; purity is unknown.

F007 CAS No. 108-20-3; diisopropyl ether; purity is unknown.
F020 241179
EOR
F002 455
F010 2.3
F004 2
F005 RE
F006 Lide D, et al. (eds.) (1997-1998). CRC Handbook of Chemistry and Physics.
* 78th Edition. CRC Press, New York, NY, USA.
F007 Lide D, et al. (eds.) (1997-1998). CRC Handbook of Chemistry and Physics.
* 78th Edition. CRC Press, New York, NY, USA.
F020 241184
EOR
F002 455
F010 2.3
F004 2
F005 RL
F006 The CRC Handbook of Chemistry and Physics is a peer reviewed publication.
* This robust summary has a reliability rating of 2 because there is
* insufficient information available on the method and analytical procedure.
F007 The CRC Handbook of Chemistry and Physics is a peer reviewed publication.
* This robust summary has a reliability rating of 2 because there is
* insufficient information available on the method and analytical procedure.
F020 241183
EOR
F002 455
F010 2.3
F004 2
F005 TS
F006 CAS No. 108-20-3; diisopropyl ether; purity is unknown.
F007 CAS No. 108-20-3; diisopropyl ether; purity is unknown.
F020 241182
EOR
F002 455
F010 2.4
F004 2
F005 ME
F006 Method not specified.
F007 Method not specified.
F020 241243
EOR
F002 455
F010 2.4
F004 2
F005 RE
F006 Daubert T and Danner R (1989). Physical and thermodynamic properties of
* pure chemicals: Data compilation. Design Institute for Physical Property
* Data, American Institute of Chemical Engineers. Hemisphere Publishing
* Corp., New York, NY, USA.
F007 Daubert T and Danner R (1989). Physical and thermodynamic properties of
* pure chemicals: Data compilation. Design Institute for Physical Property
* Data, American Institute of Chemical Engineers. Hemisphere Publishing
* Corp., New York, NY, USA.
F020 241187
EOR
F002 455
F010 2.4

F004 2
F005 RL
F006 This robust summary has a reliability rating of 2 because the data were
*   not reviewed for quality, however, the reference is from a peer-reviewed
*   handbook.
F007 This robust summary has a reliability rating of 2 because the data were
*   not reviewed for quality, however, the reference is from a peer-reviewed
*   handbook.
F020 241186
EOR
F002 455
F010 2.4
F004 2
F005 TS
F006 CAS No. 108-20-3; diisopropyl ether; purity is unknown.
F007 CAS No. 108-20-3; diisopropyl ether; purity is unknown.
F020 241185
EOR
F002 455
F010 2.5
F004 2
F005 ME
F006 Method not specified.
F007 Method not specified.
F020 241191
EOR
F002 455
F010 2.5
F004 2
F005 RE
F006 Hansch C, Leo A and Hoekman D (1995). Exploring QSAR - Hydrophobic,
*   Electronic and Steric Constants. p. 6. ACS Professional Reference Book,
*   American Chemical Society, Washington, DC, USA.
F007 Hansch C, Leo A and Hoekman D (1995). Exploring QSAR - Hydrophobic,
*   Electronic and Steric Constants. p. 6. ACS Professional Reference Book,
*   American Chemical Society, Washington, DC, USA.
F020 241194
EOR
F002 455
F010 2.5
F004 2
F005 RL
F006 The value cited by the authors is a measured and preferred value. This
*   robust summary has a reliability rating of 2 because there is
*   insufficient information available on the method and analytical procedure.
F007 The value cited by the authors is a measured and preferred value. This
*   robust summary has a reliability rating of 2 because there is
*   insufficient information available on the method and analytical procedure.
F020 241193
EOR
F002 455
F010 2.5
F004 2
F005 TS
F006 CAS No. 108-20-3; diisopropyl ether; purity is unknown.
F007 CAS No. 108-20-3; diisopropyl ether; purity is unknown.
F020 241192

EOR
F002 455
F010 2.5
F004 3
F005 RE
F006 Eadsforth C (1983). Isopropyl ether: determination of the n-octanol/water
*   partition coefficient using a reverse-phase HPLC method. Report #
*   SBGR.83.131. Shell Research Limited, Sittingbourne Research Centre,
*   Sittingbourne, Kent, England.
F007 Eadsforth C (1983). Isopropyl ether: determination of the n-octanol/water
*   partition coefficient using a reverse-phase HPLC method. Report #
*   SBGR.83.131. Shell Research Limited, Sittingbourne Research Centre,
*   Sittingbourne, Kent, England.
F020 243466
EOR
F002 455
F010 2.5
F004 3
F005 RS
F006 Log Pow = 2.4 (Pow = 250) at pH 6.7
F007 Log Pow = 2.4 (Pow = 250) at pH 6.7
F020 243464
EOR
F002 455
F010 2.5
F004 3
F005 TC
F006 The HPLC system was a reverse-phase C18-coated silica gel column, 250 mm
*   x 5 mm id, with a mobile phase of 3 volumes methanol and 1 volume water
*   (final pH 6.7) at a flow rate of 1 mL/min. 100 mL samples of an
*   approximate 1 mg/mL solution i
F007 The HPLC system was a reverse-phase C18-coated silica gel column, 250 mm
*   x 5 mm id, with a mobile phase of 3 volumes methanol and 1 volume water
*   (final pH 6.7) at a flow rate of 1 mL/min. 100 mL samples of an
*   approximate 1 mg/mL solution in the mobile phase were injected, and the
*   emergence of the material was observed using refraction index detection.
**   Thirty-one reference compounds were used to generate the linear
*   relationship between log k (k = capacity factor) and log Pow. Using the
*   HPLC retention time for the peak of the test substance, the log k was
*   determined, and the log Pow value was calculated using the linear
*   equation developed from the reference compounds.
**
**   Log Pow was determined according to the following calculations:
**   Retention time (RT), min = 5.7
**   Capacity factor, k = 0.87, k = (RTcmpd - RTunretained std)/RTunretained
*   std
**   log k = -0.06
**   linear equation: log k = -0.930 + 0.357 log Pow
F020 243465
EOR
F002 455
F010 2.6.1
F004 2
F005 RE
F006 Gerhartz W, Yamamoto Y, Kaudy L, Rounsaville J and Schulz G (eds.)
*   (1987). Ullmann's Encyclopedia of Industrial Chemistry. Vol. A 10. 5th
*   Edition. VCH Publishers, New York, NY, USA.

F007 Gerhartz W, Yamamoto Y, Kaudy L, Rounsaville J and Schulz G (eds.)
*   (1987). Ullmann's Encyclopedia of Industrial Chemistry. Vol. A 10. 5th
*   Edition. VCH Publishers, New York, NY, USA.
F020 241190
EOR
F002 455
F010 2.6.1
F004 2
F005 RL
F006 The Ullmann's Encyclopedia of Industrial Chemistry is a peer reviewed
*   publication. This robust summary has a reliability rating of 2 because
*   there is insufficient information available on the method and analytical
*   procedure.
F007 The Ullmann's Encyclopedia of Industrial Chemistry is a peer reviewed
*   publication. This robust summary has a reliability rating of 2 because
*   there is insufficient information available on the method and analytical
*   procedure.
F020 241189
EOR
F002 455
F010 2.6.1
F004 2
F005 TS
F006 CAS No. 108-20-3; diisopropyl ether; purity is unknown.
F007 CAS No. 108-20-3; diisopropyl ether; purity is unknown.
F020 241188
EOR
F002 455
F010 3.1.1
F004 2
F005 ME
F006 Calculated values using AOPWIN version 1.89, a subroutine of the computer
*   program EPIWIN version 3.12
**
**   Indirect photodegradation, or atmospheric oxidation potential, is based
*   on the structure-activity relationship methods developed by R. At
F007 Calculated values using AOPWIN version 1.89, a subroutine of the computer
*   program EPIWIN version 3.12
**
**   Indirect photodegradation, or atmospheric oxidation potential, is based
*   on the structure-activity relationship methods developed by R. Atkinson
*   under the following conditions:
**   Temperature: 25°C
**   Sensitizer: OH- radical
**   Concentration of Sensitizer: 1.5E6 OH- radicals/cm3
F020 241161
EOR
F002 455
F010 3.1.1
F004 2
F005 RE
F006 EPIWIN (2000). Estimation Program Interface for Windows, version 3.12.
*   Syracuse Research Corporation, Syracuse, NY, USA.
F007 EPIWIN (2000). Estimation Program Interface for Windows, version 3.12.
*   Syracuse Research Corporation, Syracuse, NY, USA.
F020 241164
EOR

F002 455
F010 3.1.1
F004 2
F005 RL
F006 The value was calculated based on chemical structure as modeled by
*   EPIWIN. This robust summary has a reliability rating of 2 because the
*   data are calculated and not measured.
F007 The value was calculated based on chemical structure as modeled by
*   EPIWIN. This robust summary has a reliability rating of 2 because the
*   data are calculated and not measured.
F020 241163
EOR
F002 455
F010 3.1.1
F004 2
F005 RM
F006 DIPE has the potential to volatilize to air, based on a vapor pressure of
*   19,865 Pa at 25°C (Daubert and Danner, 1989), where it is subject to
*   atmospheric oxidation. In air, DIPE can react with photosensitized oxygen
*   in the form of hydroxyl
F007 DIPE has the potential to volatilize to air, based on a vapor pressure of
*   19,865 Pa at 25°C (Daubert and Danner, 1989), where it is subject to
*   atmospheric oxidation. In air, DIPE can react with photosensitized oxygen
*   in the form of hydroxyl radicals (OH-). The computer program AOPWIN
*   (atmospheric oxidation program for Microsoft Windows) (EPIWIN, 2000)
*   calculates a chemical half-life for a 12-hour day (the 12-hour day
*   half-life value normalizes degradation to a standard day light period
*   during which hydroxyl radicals needed for degradation are generated),
*   based on an OH- reaction rate constant and a defined OH- concentration.
**   DIPE has a calculated half-life in air of 5.3 hours or 0.4 days (12-hour
*   day), based on a rate constant of 24.34 E-12 cm3/molecule*sec and an OH-
*   concentration of 1.5 E5 OH-/cm3.
F020 241162
EOR
F002 455
F010 3.1.1
F004 3
F005 ME
F006 Technical discussion
F007 Technical discussion
F020 241165
EOR
F002 455
F010 3.1.1
F004 3
F005 RE
F006 Zepp R and Cline D (1977). Rates of direct photolysis in the aqueous
*   environment. Environ. Sci. Technol. 11:359-366.
F007 Zepp R and Cline D (1977). Rates of direct photolysis in the aqueous
*   environment. Environ. Sci. Technol. 11:359-366.
F020 241167
EOR
F002 455
F010 3.1.1
F004 3
F005 RL
F006 This robust summary has a reliability of 2 because it is a technical

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*    discussion and not a study.
F007 This robust summary has a reliability of 2 because it is a technical
*    discussion and not a study.
F020 243461
EOR
F002 455
F010 3.1.1
F004 3
F005 RM
F006 Direct photochemical degradation occurs through the absorbance of solar
*    radiation by a chemical substance in aqueous solution. If the absorbed
*    energy is high enough, then the resultant excited state of the chemical
*    may undergo a transformat
F007 Direct photochemical degradation occurs through the absorbance of solar
*    radiation by a chemical substance in aqueous solution. If the absorbed
*    energy is high enough, then the resultant excited state of the chemical
*    may undergo a transformation. A prerequisite for direct photodegradation
*    is the ability of one or more bonds within a chemical to absorb
*    ultraviolet (UV)/visible light in the 290 to 750 nm range. Light
*    wavelengths longer than 750 nm do not contain sufficient energy to break
*    chemical bonds, and wavelengths below 290 nm are shielded from the earth
*    by the stratospheric ozone layer (Harris, 1982a).
**   An approach to assessing the potential for a substance to undergo
*    photochemical degradation is to assume that degradation will occur in
*    proportion to the amount of light wavelengths >290 nm absorbed by
*    constituent molecules (Zepp and Cline, 1977). The oxygen non-bonding
*    electrons in ethers do not give rise to absorption above 160 nm, which is
*    why pure ether solvents can be used in spectroscopic studies.
*    Consequently, DIPE is not subject to photolytic processes in the aqueous
*    environment.
F020 241166
EOR
F002 455
F010 3.1.2
F004 1
F005 RE
F006 Gould E (1959). Mechanism and Structure in Organic Chemistry. Holt,
*    Reinhart and Winston, New York, NY, USA.
F007 Gould E (1959). Mechanism and Structure in Organic Chemistry. Holt,
*    Reinhart and Winston, New York, NY, USA.
F020 241169
EOR
F002 455
F010 3.1.2
F004 1
F005 RE
F006 Harris J (1982). Rate of Hydrolysis. In: Handbook of Chemical Property
*    Estimation Methods. Chapter 7. Edited by WJ Lyman, WF Reehl and DH
*    Rosenblatt. McGraw-Hill Book Company, New York, NY, USA.
F007 Harris J (1982). Rate of Hydrolysis. In: Handbook of Chemical Property
*    Estimation Methods. Chapter 7. Edited by WJ Lyman, WF Reehl and DH
*    Rosenblatt. McGraw-Hill Book Company, New York, NY, USA.
F020 241170
EOR
F002 455
F010 3.1.2
F004 1
```

F005 RL
F006 This robust summary has a reliability of 2 because it is a technical
*   discussion and not a study.
F007 This robust summary has a reliability of 2 because it is a technical
*   discussion and not a study.
F020 243463
EOR
F002 455
F010 3.1.2
F004 1
F005 RS
F006 Hydrolysis of an organic chemical is the transformation process in which
*   a water molecule or hydroxide ion reacts to form a new carbon-oxygen
*   bond. Chemicals with leaving groups that have a potential to hydrolyze
*   include alkyl halides, amid
F007 Hydrolysis of an organic chemical is the transformation process in which
*   a water molecule or hydroxide ion reacts to form a new carbon-oxygen
*   bond. Chemicals with leaving groups that have a potential to hydrolyze
*   include alkyl halides, amides, carbamates, carboxylic acid esters and
*   lactones, epoxides, phosphate esters, and sulfonic acid esters (Gould,
*   1959). The lack of a suitable leaving group renders a compound resistant
*   to hydrolysis. DIPE is resistant to hydrolysis because it lacks a
*   functional group that is hydrolytically reactive and Harris (1982b)
*   identifies ether groups as generally resistant to hydrolysis. Therefore,
*   hydrolysis will not contribute to the removal of diisopropyl ether from
*   the environment.
F020 241168
EOR
F002 455
F010 3.3.1
F004 2
F005 RE
F006 Mackay D (1998). Level I Fugacity-Based Environmental Equilibrium
*   Partitioning Model, Version 2.1 (16-bit). Environmental Modelling
*   Centre, Trent University, Ontario, Canada.
F007 Mackay D (1998). Level I Fugacity-Based Environmental Equilibrium
*   Partitioning Model, Version 2.1 (16-bit). Environmental Modelling
*   Centre, Trent University, Ontario, Canada.
F020 241175
EOR
F002 455
F010 3.3.1
F004 2
F005 RL
F006 This robust summary has a reliability rating of 2 because the data are
*   calculated.
F007 This robust summary has a reliability rating of 2 because the data are
*   calculated.
F020 241174
EOR
F002 455
F010 3.3.1
F004 2
F005 RM
F006 Physicochemical data used in the calculation:
**
**   Parameter   Value w/ Units

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**
**   Molecular Weight = 102.18
**   Temperature = 25° C
**   Log Kow = 1.52
**   Water Solubility = 8,800 g/m3
**   Vapor Pressure = 19,865 Pa
**   Melting Point = -86.8° C
F007 Physicochemical data used in the calculation:
**
**   Parameter         Value w/ Units
**
**   Molecular Weight = 102.18
**   Temperature = 25° C
**   Log Kow = 1.52
**   Water Solubility = 8,800 g/m3
**   Vapor Pressure = 19,865 Pa
**   Melting Point = -86.8° C
F020 241171
EOR
F002 455
F010 3.3.1
F004 2
F005 RS
F006 Using the Mackay Level I calculation, the following
**   distribution is predicted for diisopropyl ether:
**
**   %Distribution    Compartment
**      97.83          Air
**       2.10          Water
**       0.06          Soil
**       <0.01         Sediment
**       <0.01
F007 Using the Mackay Level I calculation, the following
**   distribution is predicted for diisopropyl ether:
**
**   %Distribution    Compartment
**      97.83          Air
**       2.10          Water
**       0.06          Soil
**       <0.01         Sediment
**       <0.01         Suspended Sediment
**       <0.01         Biota
F020 241172
EOR
F002 455
F010 3.3.1
F004 2
F005 TS
F006 Diisopropyl Ether (CAS # 108-20-3)
F007 Diisopropyl Ether (CAS # 108-20-3)
F020 241173
EOR
F002 455
F010 3.3.1
F004 3
F005 CL
F006 The majority of DIPE is calculated to partition into the water phase,
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*    with smaller but significant amounts into air and soil, based on the
*    modeling parameters used in this calculation. DIPE is considered to be a
*    Type 1 chemical with potenti
F007 The majority of DIPE is calculated to partition into the water phase,
*    with smaller but significant amounts into air and soil, based on the
*    modeling parameters used in this calculation. DIPE is considered to be a
*    Type 1 chemical with potential to partition into all environmental
*    compartments.
F020 241237
EOR
F002 455
F010 3.3.1
F004 3
F005 ME
F006 Level III simulation using the Mackay Multimedia Environmental Model
*    (Mackay, 2001). Mass balances are calculated for the four bulk media of
*    air (gas + aerosol), water (solution + suspended sediment + biota), soil,
*    (solids + air + water), a
F007 Level III simulation using the Mackay Multimedia Environmental Model
*    (Mackay, 2001). Mass balances are calculated for the four bulk media of
*    air (gas + aerosol), water (solution + suspended sediment + biota), soil,
*    (solids + air + water), and sediment (solids + pore water). Equilibrium
*    exists within, but not between media. Physical-chemical properties are
*    used to quantify a chemical's behavior in an evaluative environment.
*    Three types of chemicals are treated in this model: chemicals that
*    partition into all media (Type 1), non volatile chemicals (Type 2), and
*    chemicals with zero, or near-zero, solubility (Type 3). The model can not
*    treat ionizing or speciating substances. The Level III model assumes a
*    simple, evaluative environment with user-defined volumes and densities
*    for the following homogeneous environmental media (or compartments): air,
*    water, soil, sediment, suspended sediment, fish and aerosols.
**
**   This model provides a description of a chemical's fate including the
*    important degradation and advection losses and the intermedia transport
*    processes. The distribution of the chemical between media depends on how
*    the chemical enters the system, e.g. to air, to water, or to both. This
*    mode of entry also affects persistence or residence time.
**
**   The rates of intermedia transport are controlled by a series of 12
*    transport velocities. Reaction half-lives are requested for all 7 media.
*    The advective residence time selected for air also applies to aerosols
*    and the residence time for water applies to suspended sediment and fish.
*    The advective residence time of aerosols, suspended sediment and fish
*    cannot be specified independently of the air and water residence times.
F020 241234
EOR
F002 455
F010 3.3.1
F004 3
F005 RE
F006 Mackay D (1991). Multimedia Environmental Models; The Fugacity Approach.
*    Lewis Publishers, CRC Press, pp 67-183.
F007 Mackay D (1991). Multimedia Environmental Models; The Fugacity Approach.
*    Lewis Publishers, CRC Press, pp 67-183.
F020 241239
EOR
F002 455
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F010 3.3.1
F004 3
F005 RE
F006 Mackay D (2001). Multimedia Environmental Models: The Fugacity Approach -
* Second Edition. Lewis Publishers, Boca Raton, pp.1-261.
F007 Mackay D (2001). Multimedia Environmental Models: The Fugacity Approach -
* Second Edition. Lewis Publishers, Boca Raton, pp.1-261.
F020 241242
EOR
F002 455
F010 3.3.1
F004 3
F005 RE
F006 Mackay D, et al (1996a). Assessing the fate of new and existing
* chemicals: a five-stage process. Environ. Toxicol. Chem. 15(9):1618-1626.
F007 Mackay D, et al (1996a). Assessing the fate of new and existing
* chemicals: a five-stage process. Environ. Toxicol. Chem. 15(9):1618-1626.
F020 241240
EOR
F002 455
F010 3.3.1
F004 3
F005 RE
F006 Mackay D, et al (1996b). Evaluating the environmental fate of a variety
* of types of chemicals using the EQC model. Environ. Toxicol. Chem.
* 15(9):1627-1637.
F007 Mackay D, et al (1996b). Evaluating the environmental fate of a variety
* of types of chemicals using the EQC model. Environ. Toxicol. Chem.
* 15(9):1627-1637.
F020 241241
EOR
F002 455
F010 3.3.1
F004 3
F005 RL
F006 This robust summary has a reliability rating of 2 because the data are
* calculated.
F007 This robust summary has a reliability rating of 2 because the data are
* calculated.
F020 241238
EOR
F002 455
F010 3.3.1
F004 3
F005 RS
F006 Output
** Mass% Half life(hr) Emissions(kg/hr)
** Air 19.4 25.2 1000
** Water 61.0 360 1000
** Soil 19.5 720 1000
** Sediment 0.1 3240 0
F007 Output
** Mass% Half life(hr) Emissions(kg/hr)
** Air 19.4 25.2 1000
** Water 61.0 360 1000
** Soil 19.5 720 1000
** Sediment 0.1 3240 0

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F020 241236
EOR
F002 455
F010 3.3.1
F004 3
F005 TC
F006 Physchem Inputs
**   Molar Mass = 102.18
**   Data Temperature = 25 ºC
**   Water Solubility = 8800 mg/l exp.
**   Vapour Pressure = 19865 Pa exp.
**   Log Kow = 1.52 exp.
**   Melting Point = -86.8 ºC exp.
**
**   Reaction Half Lives in hours (if not available they can be pre
F007 Physchem Inputs
**   Molar Mass = 102.18
**   Data Temperature = 25 ºC
**   Water Solubility = 8800 mg/l exp.
**   Vapour Pressure = 19865 Pa exp.
**   Log Kow = 1.52 exp.
**   Melting Point = -86.8 ºC exp.
**
**   Reaction Half Lives in hours (if not available they can be predicted
*    using EPIWIN)
**   Air (gaseous)            25.2
**   Water (no susp. part.)   360
**   Bulk Soil          720
**   Bulk Sediment            3240
**   Suspended Particles      360
**   Fish               360
**   Aerosol                        25.2
**
**   Environmental Properties (EQC standard environment)
**   Dimensions (all defaults)
**   Densities (all defaults)
**   Organic carbon & Advection (all defaults)
**   Transport Velocities (all defaults)
**
**   Emission and Inflows (defaults used)
**   Air 1000 kg/hr
**   Water 1000 kg/hr
**   Soil 1000 kg/hr
**   Sediment 0 kg/hr
F020 241235
EOR
F002 455
F010 3.3.1
F004 3
F005 TS
F006 Diisopropyl Ether, CAS No. 108-20-3
F007 Diisopropyl Ether, CAS No. 108-20-3
F020 241233
EOR
F002 455
F010 3.5
F004 2
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F005 CL
F006 Diisopropyl ether is not readily biodegradable and it did not
*   significantly inhibit the biodegradability of the test substance in an
*   inhibition test.
F007 Diisopropyl ether is not readily biodegradable and it did not
*   significantly inhibit the biodegradability of the test substance in an
*   inhibition test.
F020 241218
EOR
F002 455
F010 3.5
F004 2
F005 RE
F006 Stone C and Watkinson R (1983). Isopropyl ether: An assessment of ready
*   biodegradability. Report # SBGR.83.428. Shell Biosciences Laboratory,
*   Sittingbourne Research Centre, Sittingbourne, Kent, England.
F007 Stone C and Watkinson R (1983). Isopropyl ether: An assessment of ready
*   biodegradability. Report # SBGR.83.428. Shell Biosciences Laboratory,
*   Sittingbourne Research Centre, Sittingbourne, Kent, England.
F020 241219
EOR
F002 455
F010 3.5
F004 2
F005 RS
F006 Test substance was not readily biodegradable. After 28 days, the test
*   substance exhibited no measurable biodegradation. By day 5, >60%
*   biodegradation of positive control was observed, which meets the
*   guideline requirement. No excursions fro
F007 Test substance was not readily biodegradable. After 28 days, the test
*   substance exhibited no measurable biodegradation. By day 5, >60%
*   biodegradation of positive control was observed, which meets the
*   guideline requirement. No excursions from the testing guideline were
*   noted. The inhibition study showed that the test substance did not
*   inhibit the biodegradability of the positive control substance, sodium
*   benzoate.
**
**   % Degradation* Mean   % Degradation
**   Sample   (day 28)   (day 28)
**
**   Test Substance   0.0, 0.0   0.0
**   Na Benzoate   65.0, 73.0   69.0
**   * duplicate data
**
**   Mean oxygen concentrations (mg/L) of duplicate test systems:
**
**   Day 0
**   Mineral Salts Control = 8.85
**   Blank = 8.8
**   Na Benzoate = 8.95
**   Test Substance = 8.9 (single test system)
**   Test Substance + Na Benzoate = 8.9* (single test system)
**
**   Day 5
**   Mineral Salts Control = 9.0
**   Blank = 8.8
**   Na Benzoate = 5.7

```
**   Test Substance = 8..85
**   Test Substance + Na Benzoate = 5.8
**
**   Day 15
**   Mineral Salts Control = 8.75
**   Blank = 8.65
**   Na Benzoate = 4.9
**   Test Substance = 8.55
**   Test Substance + Na Benzoate = 4.9
**
**   Day 28
**   Mineral Salts Control = 8.65
**   Blank = 7.05
**   Na Benzoate = 3.6
**   Test Substance = 8.3
**   Test Substance + Na Benzoate = 4.15
F020 241217
EOR
F002 455
F010 3.5
F004 2
F005 TC
F006 The inoculum source was the Sittingbourne Sewage works in Kent, England,
*    and was prepared according to methods described in the OECD 301D
*    guideline. The test substance was added to the test medium by direct
*    addition at a concentration of 3.
F007 The inoculum source was the Sittingbourne Sewage works in Kent, England,
*    and was prepared according to methods described in the OECD 301D
*    guideline. The test substance was added to the test medium by direct
*    addition at a concentration of 3.0 mg/L. Test systems were incubated at
*    20 ± 1 °C and biodegradation was determined by measuring the oxygen
*    concentration on days 5, 15, and 28. Each sampling of the test substance
*    and control was conducted in duplicate. The theoretical oxygen demand was
*    2.82 mg O2 per mg test substance and a theoretical carbon dioxide (CO2)
*    evolution of 2.59 mg CO2 per mg test substance. Sodium benzoate was used
*    as the positive control.
**
**   The purity of the test substance was not supplied, but the infra-red
*    spectrum of the test substance matched a published standard (density =
*    0.723 to 0.726 kg/L). The test substance was stored in the dark at
*    ambient temperature. Nitrogen was blown over the surface of the material
*    when the container was opened and exposed to air in order to minimize
*    peroxide formation.
F020 241216
EOR
F002 455
F010 3.5
F004 3
F005 CL
F006 5-day BOD = 0.19 g/g, representing 7% biodegradation of the test
*    substance.
F007 5-day BOD = 0.19 g/g, representing 7% biodegradation of the test
*    substance.
F020 244083
EOR
F002 455
F010 3.5
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F004 3
F005 RE
F006 Bridié A, Wolff C and Winter M (1979). BOD and COD of some
* petrochemicals. Wat. Res. 13, 627-630.
F007 Bridié A, Wolff C and Winter M (1979). BOD and COD of some
* petrochemicals. Wat. Res. 13, 627-630.
F020 244085
EOR
F002 455
F010 3.5
F004 3
F005 RL
F006 The article presented a brief description of the testing methods, but
* cited a reliable guideline method in use at the time of the study.
F007 The article presented a brief description of the testing methods, but
* cited a reliable guideline method in use at the time of the study.
F020 244084
EOR
F002 455
F010 3.5
F004 3
F005 RM
F006 Test type: Biological Oxygen Demand (BOD)
F007 Test type: Biological Oxygen Demand (BOD)
F020 244108
EOR
F002 455
F010 3.5
F004 3
F005 RS
F006 0.19 g O2/g test material at 20 ± 1°C
** The theoretical oxygen demand (ThOD) of the test substance was 2.82. The
* percent ThOD in 5 days was 7%.
**
** The article stated that the only deviation from the standard method was
* the addition of 0.5 mg/
F007 0.19 g O2/g test material at 20 ± 1°C
** The theoretical oxygen demand (ThOD) of the test substance was 2.82. The
* percent ThOD in 5 days was 7%.
**
** The article stated that the only deviation from the standard method was
* the addition of 0.5 mg/L allylthiourea to prevent nitrification.
F020 244082
EOR
F002 455
F010 3.5
F004 3
F005 TC
F006 The article stated that the test method followed APHA Standard Method
* No. 219 (1971). The test was run at a temperature of 20 ± 1°C. 500-mL
* test solutions were seeded with a filtered 10-mL volume of the effluent
* from a biological sanitar
F007 The article stated that the test method followed APHA Standard Method
* No. 219 (1971). The test was run at a temperature of 20 ± 1°C. 500-mL
* test solutions were seeded with a filtered 10-mL volume of the effluent
* from a biological sanitary waste treatment plant. The activity of the
* inoculum was check by including a treatment containing a mixture of

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*    glucose and glutamic acid.  Test mixtures were stirred using a magnetic
*    stirrer.
F020 244081
EOR
F002 455
F010 3.5
F004 4
F005 CL
F006 The authors indicated that K1 values >10 L/g VSS-h represent readily
*    biodegradable organic compounds.  Based on the results of this study, all
*    three test methodologies showed the test substance to be effectively
*    utilized by activated sludge
F007 The authors indicated that K1 values >10 L/g VSS-h represent readily
*    biodegradable organic compounds.  Based on the results of this study, all
*    three test methodologies showed the test substance to be effectively
*    utilized by activated sludge microorganisms under aerobic conditions.
F020 244090
EOR
F002 455
F010 3.5
F004 4
F005 ME
F006 Comparison study of three aerobic biodegradation methods)
**   Continuous Biological Treatment:
**   (1) EPA Method 304B (EPA, 1994)
**   Batch Methods:
**   (2) Batch Oxygen addition (BOX) (Rajagopalan et al., 1998), and
**   (3) Serum Bottle Test (SBT) (Rajag
F007 Comparison study of three aerobic biodegradation methods)
**   Continuous Biological Treatment:
**   (1) EPA Method 304B (EPA, 1994)
**   Batch Methods:
**   (2) Batch Oxygen addition (BOX) (Rajagopalan et al., 1998), and
**   (3) Serum Bottle Test (SBT) (Rajagopalan et al., 1998)
F020 244086
EOR
F002 455
F010 3.5
F004 4
F005 RE
F006 Cano M, Wilcox M and van Compernolle R (1999). A direct comparison of
*    U.S. Environmental Protection Agency's Method 304B and batch tests for
*    determining activated-sludge biodegradation rate constants for volatile
*    organic compounds. Wat. Env
F007 Cano M, Wilcox M and van Compernolle R (1999). A direct comparison of
*    U.S. Environmental Protection Agency's Method 304B and batch tests for
*    determining activated-sludge biodegradation rate constants for volatile
*    organic compounds. Wat. Environ. Res. 71, 1345-1353.
F020 244092
EOR
F002 455
F010 3.5
F004 4
F005 RE
F006 Rajagopalan S, van Compernolle R, Meyer M, Cano M, and Sun P (1998).
*    Comparison of methods for determining biodegradation kinetics of volatile
*    organic compounds. Water Environ. Res. 70, 291-298.
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F007 Rajagopalan S, van Compernolle R, Meyer M, Cano M, and Sun P (1998).
*   Comparison of methods for determining biodegradation kinetics of volatile
*   organic compounds. Water Environ. Res. 70, 291-298.
F020 244094
EOR
F002 455
F010 3.5
F004 4
F005 RE
F006 U.S. EPA. (1994). Method 304B - Determination of biodegradation rates of
*   organic compounds (scrubber option). Appendix A to Part 63 - Test
*   Methods. Fed. Regist. 59,78, 19594.
F007 U.S. EPA. (1994). Method 304B - Determination of biodegradation rates of
*   organic compounds (scrubber option). Appendix A to Part 63 - Test
*   Methods. Fed. Regist. 59,78, 19594.
F020 244093
EOR
F002 455
F010 3.5
F004 4
F005 RL
F006 The publication presented a well-documented study based on ound
*   scientific principles.
F007 The publication presented a well-documented study based on ound
*   scientific principles.
F020 244091
EOR
F002 455
F010 3.5
F004 4
F005 RM
F006 Exposure Period:
**   Method 304: 30 days
**   BOX: 0.5 to 2 hours
**   SBT: 0.5 to 2 hours
F007 Exposure Period:
**   Method 304: 30 days
**   BOX: 0.5 to 2 hours
**   SBT: 0.5 to 2 hours
F020 244087
EOR
F002 455
F010 3.5
F004 4
F005 RS
F006 The average percent removal of the test substance in the continuous
*   activated sludge unit (EPA Method 304B) was 99.4%.
**
**   Three experimental trial runs with each of the three biodegradation
*   methods yielded the following average first-order bi
F007 The average percent removal of the test substance in the continuous
*   activated sludge unit (EPA Method 304B) was 99.4%.
**
**   Three experimental trial runs with each of the three biodegradation
*   methods yielded the following average first-order biodegradation rate
*   constants (K1 = L/g Volatile Suspended Solids-h) for the test substance:
**

```
**          K1 (L/g VSS-h)
**   304B         98
**   BOX          17.4
**   SBT          19.2
F020 244089
EOR
F002 455
F010 3.5
F004 4
F005 TC
F006 A pilot-scale continuous activated sludge unit served as the source of
*    biomass for kinetic rate constant comparisons of the three methods.  The
*    activated sludge was acclimated in the pilot unit by feeding a synthetic
*    cocktail of eight volat
F007 A pilot-scale continuous activated sludge unit served as the source of
*    biomass for kinetic rate constant comparisons of the three methods.  The
*    activated sludge was acclimated in the pilot unit by feeding a synthetic
*    cocktail of eight volatile organic compounds during a 2-month
*    equilibration period.  Equilibration and testing was done at ambient
*    temperature (22 to 24°C).  The hydraulic retention time (HRT) was 7.7
*    hours and the solids retention time (SRT) was 33 days.  Average organic
*    removal efficiencies based on COD and TOC were 92 and 88%, respectively.
**
**   During the biodegradation testing using Method 304B, feed and effluent
*    samples were collected in headspace-free VOA vials and stored at 4°C
*    until analyzed.  Samples were analyzed by purge-and-trap gas
*    chromatography using a flame ionization detector. Triplicate
*    biodegradation runs on the test compound were conducted with at least six
*    influent and effluent samples taken at 1 HRT (approx. 8 hours) intervals.
*
**
**   The two batch biodegradation testing methods (BOX and SBT) used activated
*    sludge biomass from the pilot-scale reactor.  Biomass was diluted using
*    effluent from the system to achieve range of 200 to 600 mg/L.  The test
*    compound was injected into the batch reactors and the concentration was
*    monitored over time by collecting gas samples directly from the headspace
*    using an automatic sampling pump and analyzing immediately using gas
*    chromatography.
F020 244088
EOR
F002 455
F010 3.5
F004 5
F005 CL
F006 Diisopropyl ether can be effectively biodegraded in high biomass aerobic
*    reactors.
F007 Diisopropyl ether can be effectively biodegraded in high biomass aerobic
*    reactors.
F020 244098
EOR
F002 455
F010 3.5
F004 5
F005 RE
F006 Pruden A, Suidan M, Venosa A and Wilson G (2001). Biodegradaton of methyl
*    tert-butyl ether under various substrate conditions. Environ. Sci.
*    Technol. 35, 4235-4241.
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F007 Pruden A, Suidan M, Venosa A and Wilson G (2001). Biodegradaton of methyl
*   tert-butyl ether under various substrate conditions. Environ. Sci.
*   Technol. 35, 4235-4241.
F020 244100
EOR
F002 455
F010 3.5
F004 5
F005 RL
F006 The report provided adequate details of the test conditions but reported
*   only a text description of biodegradation results.
F007 The report provided adequate details of the test conditions but reported
*   only a text description of biodegradation results.
F020 244099
EOR
F002 455
F010 3.5
F004 5
F005 RM
F006 Inoculum consisted of a mixture of the following:
**   1) mixed liquor from the Metropolitan Sewer District (MSD), Cincinnati,
*   OH,
**   2) mixed liquor from Shell Development Co., Houston, TX, and
**   3) aquifer material wash water from a MTBE-contaminat
F007 Inoculum consisted of a mixture of the following:
**   1) mixed liquor from the Metropolitan Sewer District (MSD), Cincinnati,
*   OH,
**   2) mixed liquor from Shell Development Co., Houston, TX, and
**   3) aquifer material wash water from a MTBE-contaminated site in Port
*   Hueneme, CA.
F020 244095
EOR
F002 455
F010 3.5
F004 5
F005 RS
F006 The authors indicated that removal of DIPE was comparable to that
*   achieved for MTBE, which was greater than 99.9%.
F007 The authors indicated that removal of DIPE was comparable to that
*   achieved for MTBE, which was greater than 99.9%.
F020 244097
EOR
F002 455
F010 3.5
F004 5
F005 TC
F006 Bioreactors (Autoclave Engineers, Erie, PA) were initially seeded with 2
*   L of mixed liquor from the MSD, 600 mL of mixed liquor from Shell
*   Development Co., and 140 mL of aquifer wash water. Cultures were
*   maintained on a total influent feed
F007 Bioreactors (Autoclave Engineers, Erie, PA) were initially seeded with 2
*   L of mixed liquor from the MSD, 600 mL of mixed liquor from Shell
*   Development Co., and 140 mL of aquifer wash water. Cultures were
*   maintained on a total influent feed of 417 mg/L chemical oxygen demand
*   (COD) divided as 50% methyl tert-butyl ether (MTBE) and 50% as
*   diisopropyl ether (DIPE).
**

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**   Reactors were well mixed and controlled to a temperature of 20°C.  To
*    retain high biomass levels, a polyethylene porous pot was inserted into
*    the reactor.  The pots consisted of 0.45 cm thick filter-grade
*    polyethylene (pore size = 20 mm), with an internal diameter of 19.1 cm
*    and a height of 29.2 cm. Initially, a solids retention time of 18 days
*    was maintained by wasting intentionally from the reactor.  Subsequently
*    (after about 120 days) intentional wasting ceased and only took place
*    during sampling of the reactors.
**
**   The combined influent flow rate was 2.37 L/d, with 80% of the total flow
*    provided by a pH-adjustment solution, and 20% provided by an acidified
*    nutrient solution.  The pH-adjustment solutions contained deionized
*    water, MTBE and DIPE fed by a syringe infusion pump, and an appropriate
*    amount of 10N sodium hydroxide to maintain the pH between 7.4 and 8.0.
*    The nutrient solution consisted of deionized water with essential salts
*    and vitamins added to promote biological growth.  Final nutrient
*    concentrations inside the reactor were as follows: (NH4)2SO4, 93 mg/L;
*    MgSO4, 69.6 mg/L; CaCl2o2H2O, 22.5 mg/L; K2HPO4, 6.9 mg/L; CuSO4oH2O,
*    0.08 mg/L; Na2MoO4o2H2O, 0.15 mg/L; MnSO4oH2O, 0.13 mg/L; ZnCl2, 0.23
*    mg/L; CoCl2o6H2O, 0.42 mg/L; and FeCl2o4H2O, 17.25 mg/L..  The hydraulic
*    retention time was 4.2 days with a total reactor volume of 9.95 L and an
*    enrichment culture volume of 6 L.
**
**   Effluent from the reactors was monitored weekly for the presence of MTBE
*    and DIPE using gas chromatography equipped with a flame ionization
*    detector (FID) and a 60/80 Carbopack B5% Carbowax 20 M glass column. The
*    pH of the system was measured daily, and COD and dissolved organic carbon
*    (DOC)  was measured weekly.
F020 244096
EOR
F002 455
F010 3.5
F004 6
F005 CL
F006 The test substance was not aerobically biodegraded by indigenous
*    subsurface microflora.
F007 The test substance was not aerobically biodegraded by indigenous
*    subsurface microflora.
F020 244104
EOR
F002 455
F010 3.5
F004 6
F005 RE
F006 Zenker M, Borden R, and Barlaz M (1999). Investigation of the intrinsic
*    biodegradation of alkyl and cyclic ethers. Vol. 1, pp 165-170, 5th Int.
*    In Situ On-Site Biorem. Symp.
F007 Zenker M, Borden R, and Barlaz M (1999). Investigation of the intrinsic
*    biodegradation of alkyl and cyclic ethers. Vol. 1, pp 165-170, 5th Int.
*    In Situ On-Site Biorem. Symp.
F020 244106
EOR
F002 455
F010 3.5
F004 6
F005 RL
F006 The testing method did not follow any specific regulatory guideline
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*    method, but the publication provided valuable information using sound
*    scientific principles.
F007 The testing method did not follow any specific regulatory guideline
*    method, but the publication provided valuable information using sound
*    scientific principles.
F020 244105
EOR
F002 455
F010 3.5
F004 6
F005 RM
F006 Test type:  soil/water microcosm
F007 Test type:  soil/water microcosm
F020 244103
EOR
F002 455
F010 3.5
F004 6
F005 RS
F006 No detectable biodegradation of the test substance occurred after one
*    year of incubation.
F007 No detectable biodegradation of the test substance occurred after one
*    year of incubation.
F020 244102
EOR
F002 455
F010 3.5
F004 6
F005 TC
F006 Soil and water from an aquifer with previous exposure to methyl
*    tert-butyl ether (MTBE) was collected using a coring device and a pump.
*    The material was brought to the laboratory where the sediment was
*    thoroughly mixed.  Groundwater was fi
F007 Soil and water from an aquifer with previous exposure to methyl
*    tert-butyl ether (MTBE) was collected using a coring device and a pump.
*    The material was brought to the laboratory where the sediment was
*    thoroughly mixed.  Groundwater was filtered through a 0.45 mm filter and
*    sparged for 12 hours with sterile air to oxygenate the water and to
*    remove background volatile chemicals.  Analysis by gas chromatography
*    indicated that concentrations of MTBE in the aqueous samples were <10
*    mg/L.  Microcosms were constructed in amber 255-mL screw-top bottles
*    sealed with TeflonÒ MininertÒ valves. Each bottle contained 150 g of wet
*    sediment, 140 mL of sterile groundwater and 3000 mg/L of diisopropyl
*    ether (DIPE).  Treatments were constructed in triplicate with matching
*    abiotic controls.  Sediment used for the abiotic controls was autoclaved
*    for one hour on each of three consecutive days.  Additionally, 250 mg/L
*    of mercuric chloride was added to ensure no biological activity.
*    Microcosms were incubated in the dark at 16 °C.
**
**   All samples were analyzed every 30 days by purge and trap gas
*    chromatography and flame ionization detection to determine concentrations
*    of the test substance.  Test substance disappearance relative to abiotic
*    controls was the principal indicator of biodegradation.
F020 244101
EOR
F002 455
F010 3.5
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F004 7
F005 CL
F006 Diisopropyl ether was a persistent molecule that resisted anaerobic
* destruction. After 252 days, no evidence for the anaerobic
* biodegradability of diisopropyl ether was obtained.
F007 Diisopropyl ether was a persistent molecule that resisted anaerobic
* destruction. After 252 days, no evidence for the anaerobic
* biodegradability of diisopropyl ether was obtained.
F020 244111
EOR
F002 455
F010 3.5
F004 7
F005 RE
F006 Suflita J and Mormile M (1993). Anaerobic biodegradation of known and
* potential gasoline oxygenates in the terrestrial subsurface. Environ.
* Sci. Technol. 27, 976-978.
F007 Suflita J and Mormile M (1993). Anaerobic biodegradation of known and
* potential gasoline oxygenates in the terrestrial subsurface. Environ.
* Sci. Technol. 27, 976-978.
F020 244113
EOR
F002 455
F010 3.5
F004 7
F005 RL
F006 The publication reported a well-documented study that meets basic
* scientific principles.
F007 The publication reported a well-documented study that meets basic
* scientific principles.
F020 244112
EOR
F002 455
F010 3.5
F004 7
F005 RS
F006 Biodegradation Rate (ppm C/day) = 0
** Methane recovery (% theoretical) = 0
F007 Biodegradation Rate (ppm C/day) = 0
** Methane recovery (% theoretical) = 0
F020 244110
EOR
F002 455
F010 3.5
F004 7
F005 TC
F006 Diisopropyl ether was tested for the ability of the compound to be
* completely biodegraded to methane in an aquifer slurry. Sediment and
* groundwater were collected from a methanogenic portion of a shallow
* anoxic aquifer polluted by municipal
F007 Diisopropyl ether was tested for the ability of the compound to be
* completely biodegraded to methane in an aquifer slurry. Sediment and
* groundwater were collected from a methanogenic portion of a shallow
* anoxic aquifer polluted by municipal landfill leachate. Slurries were
* prepared by placing 50 g of sediment and 75 mL of groundwater in sterile
* 160-mL serum bottles. The bottles were sealed with Teflon-lined stoppers
* and incubated in the dark at room temperature. Diisopropyl ether was

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*    added to the incubation mixture to reach an initial substrate
*    concentration of 50 ppm C.  Pressure increases resulting from biogas
*    formation (CH4 and CO2) were monitored with an automated pressure
*    transducer system. The acclimation time was estimated as the amount of
*    time where no significant pressure difference was measured between the
*    substrate-amended treatment and un-amended controls.
**
**   At the end of the incubation period, biodegradation was measured as the
*    depletion of parent substrate and the formation of methane over
*    background controls.  Measurements were made using gas chromatography
*    equipped with a flame ionization detector.  A 1.8 m x 0.32 cm 80/100
*    porapak Q column or a 0.2% Carbowax 1500 on Carbopack C column were used
*    for headspace methane analyses and test substance determinations,
*    respectively.  Autoclaved controls were similarly assayed and were
*    uniformly unable to exhibit methane formation or test substance
*    disappearance.  The amount of methane formed in aquifer incubations was
*    compared to that theoretically expected based on the Buswell equation.
F020 244109
EOR
F002 455
F010 3.5
F004 8
F005 CL
F006 Diisopropyl ether is not anaerobically degraded under nitrate- or
*    sulfate-reducing conditions, and it is not anaerobically degraded under
*    methanogenic conditions.
F007 Diisopropyl ether is not anaerobically degraded under nitrate- or
*    sulfate-reducing conditions, and it is not anaerobically degraded under
*    methanogenic conditions.
F020 244117
EOR
F002 455
F010 3.5
F004 8
F005 RE
F006 Mormile M, Liu S and Suflita J (1994). Anaerobic biodegradation of
*    gasoline oxygenates: Extrapolation of information to multiple sites and
*    redox conditions. Environ. Sci. Technol. 28, 1727-1732.
F007 Mormile M, Liu S and Suflita J (1994). Anaerobic biodegradation of
*    gasoline oxygenates: Extrapolation of information to multiple sites and
*    redox conditions. Environ. Sci. Technol. 28, 1727-1732.
F020 244119
EOR
F002 455
F010 3.5
F004 8
F005 RL
F006 The publication reported a well-documented study that meets basic
*    scientific principles.
F007 The publication reported a well-documented study that meets basic
*    scientific principles.
F020 244118
EOR
F002 455
F010 3.5
F004 8
F005 RM
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F006 Exposure period: 85, 180, or 244 days
F007 Exposure period: 85, 180, or 244 days
F020 244114
EOR
F002 455
F010 3.5
F004 8
F005 RS
F006 Biodegradation of diisopropyl ether with sulfate or nitrate available as
*   electron acceptors:
**
**   SO4 or NO3
**   Substrate Amount Consumed   Rate
**   Loss (%) (% Theoretical) (umol/SO4/
F007 Biodegradation of diisopropyl ether with sulfate or nitrate available as
*   electron acceptors:
**
**   SO4 or NO3
**   Substrate Amount Consumed   Rate
**   Loss (%) (% Theoretical) (umol/SO4/day)
**   sulfate-reducing   0   0   0
**   nitrate-reducing   0   0   0
**
**
**   Biodegradation of diisopropyl ether under methanogenic conditions:
**   Degradation   Methane Recovery
**   Rate (ppm C/day)   (% Expected)
**   Fuel-impacted river
**   sediment   0   0
**   Industrial/sewage
**   impacted creek sediment   0   6
F020 244116
EOR
F002 455
F010 3.5
F004 8
F005 TC
F006 Several tests were carried out to determine the anaerobic biodegradation
*   of the test substance. Three experiments were done to determine
*   biodegradation under sulfate- and nitrate-reducing conditions and under
*   methanogenic conditions. Sedi
F007 Several tests were carried out to determine the anaerobic biodegradation
*   of the test substance. Three experiments were done to determine
*   biodegradation under sulfate- and nitrate-reducing conditions and under
*   methanogenic conditions. Sediment and surface water (or groundwater)
*   from three sources were used as inoculum in separate experiments; (1)
*   sediment/groundwater from a landfill leachate impacted aquifer, (2)
*   sediment/surface water from a river historically impacted by oil storage
*   and barge loading facilities, and (3) sediment/surface water from a creek
*   impacted by industrial waste and domestic sewage sludge.
**
**   Slurries were prepared by placing 50 g of sediment and 75 mL of water
*   into sterile 160-mL serum bottles. Water was amended with sodium sulfide
*   (1 mM) and resazurin (0.0002%) to serve as reductant and redox indicator,
*   respectively. The bottles were sealed with stoppers and the headspace
*   above the slurries was adjusted to 80% N2:20%CO2 (1 atm). To the landfill
*   leachate-impacted samples, either sodium sulfate (5mM) or sodium nitrate

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*    (8 mM) was added in order to assess potential test substance decay
*    coupled with the consumption of these electrons (referred to as
*    sulfate-reducing and nitrate-reducing incubations, respectively). The
*    test substance was added to the slurries to give an initial concentration
*    of 50 ppm C.  The rates of methane production, sulfate reduction, and
*    nitrate depletion were monitored in slurries receiving the test substance
*    and compared to test substance-free controls.  All incubations were done
*    in the dark at 24°C.  The sulfate-reducing experiment was run for 244
*    days, the nitrate-reducing experiment was run for 85 days, and the
*    methanogenic experiment was run for 180 days.
**
**   In the methanogenic incubations, increases in headspace pressure were
*    routinely monitored.  Parent compound depletion and formation of methane
*    were confirmed by gas chromatography (GC).  The net amount of sulfate and
*    nitrate depletion over the controls was monitored by high pressure liquid
*    chromatrography (HPLC).
F020 244115
EOR
F002 455
F010 3.5
F004 9
F005 CL
F006 Diisopropyl ether was degraded by 78% within 24 hours.
F007 Diisopropyl ether was degraded by 78% within 24 hours.
F020 244122
EOR
F002 455
F010 3.5
F004 9
F005 RE
F006 Hernandez-Perez G, Fayolle F and Vandecasteele J-P (2001). Biodegradation
*    of ethyl t-butyl ether (ETBE), methyl t-butyl ether (MTBE) and t-amyl
*    methyl ether (TAME) by Gordonia terrae. Appl. Microbiol. Biotechnol. 55,
*    117-121.
F007 Hernandez-Perez G, Fayolle F and Vandecasteele J-P (2001). Biodegradation
*    of ethyl t-butyl ether (ETBE), methyl t-butyl ether (MTBE) and t-amyl
*    methyl ether (TAME) by Gordonia terrae. Appl. Microbiol. Biotechnol. 55,
*    117-121.
F020 244124
EOR
F002 455
F010 3.5
F004 9
F005 RL
F006 Information on the analytical method was not provided in the report.
F007 Information on the analytical method was not provided in the report.
F020 244123
EOR
F002 455
F010 3.5
F004 9
F005 RS
F006 Diisopropyl ether was degraded by 78% over the 24-hour incubation period.
**
**   Comparison of DIPE biodegradation to ETBE:
**      Test Substance  Degradation (%)
**           ETBE              100
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**
**   The authors indicated concentrations of the test substanc
F007 Diisopropyl ether was degraded by 78% over the 24-hour incubation period.
**
**   Comparison of DIPE biodegradation to ETBE:
**      Test Substance  Degradation (%)
**           ETBE              100
**
**   The authors indicated concentrations of the test substance in the flasks
*    were quantified by analytical means. The method was not described in the
*    report, but was referenced in an earlier publication by the same workers.
F020 244121
EOR
F002 455
F010 3.5
F004 9
F005 TC
F006 The capacity of ethyl t-butyl ether (ETBE)-induced resting cells of the
*    inoculum to degrade diisopropyl ether was tested in sealed flasks. The
*    article focused on biodegradation of ETBE, methyl t-butyl ether (MTBE)
*    and t-amyl methyl ether (T
F007 The capacity of ethyl t-butyl ether (ETBE)-induced resting cells of the
*    inoculum to degrade diisopropyl ether was tested in sealed flasks. The
*    article focused on biodegradation of ETBE, methyl t-butyl ether (MTBE)
*    and t-amyl methyl ether (TAME), but was tested on other ethers including
*    diisopropyl ether (DIPE).
**
**   G. terrae IFP 2001 was cultivated on ETBE-supplemented MM medium.  After
*    24 hours incubation, bacteria were harvested by centrifugation (20,000 g
*    for 20 minutes), washed twice in 100 mM Tris-HCl buffer at pH 7.0 and
*    re-suspended in Tris-HCl.  The test substance was added to 20-mL cell
*    suspensions in 125-mL sealed flasks.  Flasks were incubated for 24 hours
*    at 30 °C with orbital shaking.  Initial cell concentration was 0.5 g/L.
*    The test substance was tested at 100 mg/L.  Filtered samples were
*    analyzed at 0-hour and 24-hours.
F020 244120
EOR
F002 455
F010 3.7
F004 1
F005 RE
F006 EPI SuiteTM (2000). Estimation Program Interface Suite, v3.12. Syracuse
*    Research Corporation, Syracuse, NY, USA.
F007 EPI SuiteTM (2000). Estimation Program Interface Suite, v3.12. Syracuse
*    Research Corporation, Syracuse, NY, USA.
F020 243383
EOR
F002 455
F010 3.7
F004 1
F005 RL
F006 This robust summary has a reliability rating of 2 because the data are
*    calculated and not measured.
F007 This robust summary has a reliability rating of 2 because the data are
*    calculated and not measured.
F020 243382
EOR
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F002 455
F010 3.7
F004 1
F005 RM
F006 A log bioconcentration factor (BCF) of 0.47 is calculated (BCF = 2.95).
* With respect to a log Kow = 1.52, which was used to calculate the BCF,
* diisopropyl ether in the aquatic environment is expected to have a low
* bioaccumulation potential.
F007 A log bioconcentration factor (BCF) of 0.47 is calculated (BCF = 2.95).
* With respect to a log Kow = 1.52, which was used to calculate the BCF,
* diisopropyl ether in the aquatic environment is expected to have a low
* bioaccumulation potential.
F020 243381
EOR
F002 455
F010 3.7
F004 2
F005 RE
F006 EPI SuiteTM (2000). Estimation Program Interface Suite, v3.12. Syracuse
* Research Corporation, Syracuse, NY, USA.
F007 EPI SuiteTM (2000). Estimation Program Interface Suite, v3.12. Syracuse
* Research Corporation, Syracuse, NY, USA.
F020 243469
EOR
F002 455
F010 3.7
F004 2
F005 RL
F006 This robust summary has a reliability rating of 2 because the data are
* calculated and not measured.
F007 This robust summary has a reliability rating of 2 because the data are
* calculated and not measured.
F020 243468
EOR
F002 455
F010 3.7
F004 2
F005 RM
F006 A log bioconcentration factor (BCF) of 1.15 is calculated (BCF = 14.06).
* With respect to a log Kow = 2.4, which was used to calculate the BCF,
* disiopropyl ether in the aquatic environment is expected to have a low
* bioaccumulation potential.
F007 A log bioconcentration factor (BCF) of 1.15 is calculated (BCF = 14.06).
* With respect to a log Kow = 2.4, which was used to calculate the BCF,
* disiopropyl ether in the aquatic environment is expected to have a low
* bioaccumulation potential.
F020 243467
EOR
F002 455
F010 3.8
F004 1
F005 RE
F006 Church C and Tratnyek P (2000). Process level investigations of the in
* situ degradation of MTBE. Presented at the MTBE Biodegradation Workshop,
* February 1-3, 2000. Cincinnati, OH, USA.
F007 Church C and Tratnyek P (2000). Process level investigations of the in
* situ degradation of MTBE. Presented at the MTBE Biodegradation Workshop,

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*    February 1-3, 2000. Cincinnati, OH, USA.
F020 244127
EOR
F002 455
F010 3.8
F004 1
F005 RE
F006 Eastern Research Group Inc. (2001). Summary of Workshop on Biodegradation
*    of MTBE, February 1-3, 2000.  Report No. EPA/625/R-01/001A, February,
*    2001.
F007 Eastern Research Group Inc. (2001). Summary of Workshop on Biodegradation
*    of MTBE, February 1-3, 2000.  Report No. EPA/625/R-01/001A, February,
*    2001.
F020 244126
EOR
F002 455
F010 3.8
F004 1
F005 RE
F006 Kropp K, Mormile M and Suflita J (2000). Anaerobic biodegradation of MTBE
*    and alternative gasoline oxygenates. Presented at the MTBE Biodegradation
*    Workshop, February 1-3, 2000. Cincinnati, OH, USA.
F007 Kropp K, Mormile M and Suflita J (2000). Anaerobic biodegradation of MTBE
*    and alternative gasoline oxygenates. Presented at the MTBE Biodegradation
*    Workshop, February 1-3, 2000. Cincinnati, OH, USA.
F020 244128
EOR
F002 455
F010 3.8
F004 1
F005 RE
F006 Scow K, Smith A, Leung J, Mackay D and Lory E (2000). Bioaugmentation of
*    MTBE-contaminated groundwater with bacterial strain PM1. Presented at the
*    MTBE Biodegradation Workshop, February 1-3, 2000. Cincinnati, OH, USA.
F007 Scow K, Smith A, Leung J, Mackay D and Lory E (2000). Bioaugmentation of
*    MTBE-contaminated groundwater with bacterial strain PM1. Presented at the
*    MTBE Biodegradation Workshop, February 1-3, 2000. Cincinnati, OH, USA.
F020 244129
EOR
F002 455
F010 3.8
F004 1
F005 RM
F006 The article reports on a U.S EPA and American Petroleum Institute
*    workshop (February 1-3, 2000) on biodegradation of methyl tert-butyl
*    ether (MTBE)-contaminated soils and groundwater.  MTBE is one of a group
*    of structurally similar compound
F007 The article reports on a U.S EPA and American Petroleum Institute
*    workshop (February 1-3, 2000) on biodegradation of methyl tert-butyl
*    ether (MTBE)-contaminated soils and groundwater.  MTBE is one of a group
*    of structurally similar compounds commonly called alkyl ether oxygenates
*    (AEO) that are added to reformulated gasoline to reduce carbon monoxide
*    and ozone emissions.  Diisopropyl ether (DIPE) is one type of AEO that is
*    used in gasoline along others in this class of chemicals.  The workshop
*    focused on the status of the current research and understanding on
*    biodegradation of MTBE and reported relevant information on the
*    biodegradation of DIPE and other AEOs used in reformulated gasoline.
```

**
** Pure microbial cultures have been identified and isolated that have
*   demonstrated the capability of utilizing MTBE as a sole carbon and energy
*   source under aerobic conditions (Scow et al., 2000). This isolate,
*   bacterial strain PM1, was studied by Church and Tratnyek (2000) to
*   determine the aerobic degradation pathway of MTBE. In their study, the
*   authors confirmed the mineralization of MTBE and determined the
*   degradation rates of DIPE and other AEOs were of the same order of
*   magnitude as the degradation rates of MTBE (Church and Tratnyek, 2000).
*   Their results suggested that similar enzyme systems were responsible for
*   all of the reactions.
**
** While the majority of research on anaerobic biodegradation of these
*   compounds has been unable to show that MTBE is utilized, a few studies
*   have demonstrated that MTBE and other AEOs may be susceptible to attack
*   under anaerobic conditions. Kropp et al. (2000) studied the anaerobic
*   biodegradation potential of MTBE, DIPE, and other oxygenates in sediment
*   slurries under methanogenic conditions. They found definite evidence in
*   the form of methane and carbon dioxide production to conclude that
*   anaerobic degradation was occurring. The workshop authors concluded that
*   anaerobic biodegradation was a phenomena that was not widespread and
*   extremely difficult for these compounds.
F020 244125
EOR
F002 455
F010 3.8
F004 2
F005 RM
F006 Diisopropyl ether (DIPE) is one of a group of similar compounds referred
*   to as alkyl ether oxygenates (AEO) that are added to reformulated
*   gasoline. Biodegradation studies with DIPE and other AEO compounds have
*   demonstrated the ability of t
F007 Diisopropyl ether (DIPE) is one of a group of similar compounds referred
*   to as alkyl ether oxygenates (AEO) that are added to reformulated
*   gasoline. Biodegradation studies with DIPE and other AEO compounds have
*   demonstrated the ability of these substances to be consumed by pure
*   strains and mixed cultures of bacteria when incubated under aerobic
*   conditions. Church and Tratnyek (2000) showed that bacterial strain PM1,
*   which had been acclimated to methyl t-butyl ether (MTBE), could
*   mineralize MTBE and demonstrated similar degradation rates for DIPE and
*   other AEOs. They concluded that similar enzymes were responsible for all
*   the degradation reactions. Additional evidence showing the wide spectrum
*   of activity of the bacterial enzyme systems to degrade AEOs was provided
*   by Hernandez-Perez et al. (2001). Using isolated Gordonia terrae (strain
*   IFP 2001) that had been grown on ethyl t-butyl ether (ETBE), degradation
*   of a variety of other AEOs could be achieved. DIPE was degraded 78%
*   within 24 hours in their study (Hernandez-Perez et al. 2001).
**
** Optimum biodegradation in mixed culture systems occurred when the
*   microbial culture is allowed a period of acclimation to the substrate.
*   For example, Bridié et al. (1979) measured only 7% consumption of the
*   theoretical oxygen demand when DIPE was tested in a 5-day BOD test. In
*   contrast, Cano et al. (1999) showed rapid utilization of DIPE when
*   activated sludge was conditioned to a cocktail of volatile organic
*   compounds for two months. In a continuous flow reactor, DIPE removal
*   averaged 99.4%. Cano et al. (1999) also measured high rates of
*   biodegradation of DIPE when comparing the continuous treatment method

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*    (EPA Method 304B) (EPA, 1994) to two batch treatment methods (BOX and SBT
*    methods; Rajagopalan et al., 1998). Based on the measured rate constants,
*    the authors considered DIPE to be readily biodegradable. Pruden et al.
*    (2001) also observed high removal rates (e.g., 99.9%) of DIPE through a
*    continuous flow reactor system. The performance of the reactors was
*    enhanced when biomass was retained in the reactor, suggesting that a long
*    biomass residence time may be needed for complete mineralization.
**
**   Biodegradation of DIPE is not always observed in biodegradation assays.
*    Zenker et al. (1999) failed to show biodegradation of DIPE over a 1-year
*    period using indigenous microflora in sediment and water from an aquifer
*    that had been previously exposed to MTBE. Given the apparent need of
*    microbial communities for a period of acclimation to DIPE, it is unlikely
*    that DIPE would be considered readily biodegradable in standard guideline
*    studies. However, the evidence shows that DIPE can be inherently degraded
*    by pure strains of bacteria and mixed enrichments of activated sludge
*    microorganisms.
**
**   While available research shows that DIPE is capable of being biodegraded
*    under aerobic conditions, anaerobic biodegradation is extremely difficult
*    and this substance is considered recalcitrant under those conditions.
*    Suflita et al. (1993) showed no biodegradation of DIPE after 252 days of
*    anaerobic incubation. Substrate was added as 50 ppm C to sediment and
*    groundwater collected from a methanogenic portion of a shallow anoxic
*    aquifer. Similarly, DIPE was evaluated for anaerobic biodegradability
*    under methanogenic conditions as well as sulfate and nitrate-reducing
*    conditions (Mormile et al., 1994). Inocula from three sources (e.g.,
*    sediment/groundwater from an aquifer impacted by landfill leachate,
*    sediment/surface water from a river impacted by oil storage, and
*    sediment/surface water from a creek impacted by industrial waste and
*    domestic sewage) were used in separate incubations to assess anaerobic
*    biodegradation in sealed serum bottles. No DIPE biodegradation was
*    measured over incubation periods of 85 days (nitrate-reducing
*    conditions), 180 days (methanogenic conditions), and 244 days
*    (sulfate-reducing conditions). Lack of methane production reported by
*    Suflita and Mormile (1993) does not preclude partial anaerobic
*    biodegradation of DIPE in their studies because only methane was
*    monitored. Kropp et al. (2000) studied the anaerobic biodegradation
*    potential of a number of AEOs including DIPE in sediment slurries under
*    methanogenic conditions.  They found evidence in the form of methane and
*    carbon dioxide production to conclude that anaerobic biodegradation was
*    occurring, although the authors stated that anaerobic biodegradation was
*    not a widespread phenomena and extremely difficult for these compounds.
F020 244130
EOR
F002 455
F010 4.1
F004 1
F005 CL
F006 96-hour LC50 = 91.7 mg/L based upon measured values.
F007 96-hour LC50 = 91.7 mg/L based upon measured values.
F020 241341
EOR
F002 455
F010 4.1
F004 1
F005 ME
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F006 The water solubility of the test chemical was obtained from literature or
*   determined experimentally. A flow through system using proportional
*   diluters and modified continuous mini-diluter system was used for
*   maintaining the required test co
F007 The water solubility of the test chemical was obtained from literature or
*   determined experimentally. A flow through system using proportional
*   diluters and modified continuous mini-diluter system was used for
*   maintaining the required test concentrations
**
**   Twenty to twenty-five 30 day-old fish, each weighing approximately 0.12
*   g, were randomly divided amongst the test tanks (control and five
*   different concentrations) with flow-through dilutor systems.
**
**   Lake Superior water maintained at 25°C ± 1°C was used in the test.
*   Routine measures of hardness (EDTA) and total alkalinity of test water
*   yielded mean values of 45.5 and 42.2 mg/L as CaCO3, respectively. The
*   arithmetic mean of the pH was 7.5 and dissolved oxygen was always greater
*   than 60% of saturation.
**
**   Fish were supplied from the United States Environmental Protection
*   Agency, Environmental Research Laboratory-Duluth culture. They were not
*   fed during the test. Deaths were recorded after 1, 3, 6,12, 24, 48, 72,
*   and 96 hours.
F020 241339
EOR
F002 455
F010 4.1
F004 1
F005 RE
F006 Veith G, Call D and Brooke L (1983). Structure-Toxicity Relationships for
*   the Fathead Minnow, Pimephales promelas: Narcotic Industrial Chemicals.
*   Can. J. Fish. Aquat. Sci. 40, 743-748.
F007 Veith G, Call D and Brooke L (1983). Structure-Toxicity Relationships for
*   the Fathead Minnow, Pimephales promelas: Narcotic Industrial Chemicals.
*   Can. J. Fish. Aquat. Sci. 40, 743-748.
F008 HEDSET
F009 19-10-1993
F020 235979
EOR
F002 455
F010 4.1
F004 1
F005 RL
F006 This robust summary has a reliability rating of 2 because complete
*   information on the analytical results were not available and the study
*   was not conducted under GLP.
F007 This robust summary has a reliability rating of 2 because complete
*   information on the analytical results were not available and the study
*   was not conducted under GLP.
F020 241342
EOR
F002 455
F010 4.1
F004 1
F005 RM
F006 Statistics: Trimmed Spearman-Karber Method
F007 Statistics: Trimmed Spearman-Karber Method

F020 241343
EOR
F002 455
F010 4.1
F004 1
F005 RM
F006 Test method described in reference.
F007 Test method described in reference.
F008 HEDSET
F009 19-10-1993
F020 235978
EOR
F002 455
F010 4.1
F004 1
F005 RS
F006 96-hour LL50 = 91.7 mg/L based upon measured values
**
** Analytical method used was GC analysis with Flame Ionization Detection
*   (GC-FID), performed on a Hewlett-Packard model 5730A gas chromatograph.
*   Concentrations of the test chemical were mea
F007 96-hour LL50 = 91.7 mg/L based upon measured values
**
** Analytical method used was GC analysis with Flame Ionization Detection
*   (GC-FID), performed on a Hewlett-Packard model 5730A gas chromatograph.
*   Concentrations of the test chemical were measured daily at each exposure
*   level.
F020 241340
EOR
F002 455
F010 4.1
F004 2
F005 CL
F006 The predicted 96 h LC50 value for fish (214.1 mg/L) is in good agreement
*   with the experimental 96 h LC50 value for fathead minnow (Pimephales
*   promelas) (91.7 mg/L) (Veith et al., Can. J. Fish. Aquat. Sci.,
*   40:743-748) and 48 h EC50 value fo
F007 The predicted 96 h LC50 value for fish (214.1 mg/L) is in good agreement
*   with the experimental 96 h LC50 value for fathead minnow (Pimephales
*   promelas) (91.7 mg/L) (Veith et al., Can. J. Fish. Aquat. Sci.,
*   40:743-748) and 48 h EC50 value for Daphnia (190.0 mg/L) (Stephenson
*   R.R., Shell Research Limited, Report No. SBGR.83.215).
F020 241204
EOR
F002 455
F010 4.1
F004 2
F005 ME
F006 ECOSAR version 0.99h, US EPA. The structure-activity relationships (SARs)
*   presented in this program are used to predict the aquatic toxicity of
*   chemicals based on their similarity of structure to chemicals for which
*   the aquatic toxicity has
F007 ECOSAR version 0.99h, US EPA. The structure-activity relationships (SARs)
*   presented in this program are used to predict the aquatic toxicity of
*   chemicals based on their similarity of structure to chemicals for which
*   the aquatic toxicity has been previously measured. Most SAR calculations
*   in the ECOSAR Class Program are based upon the octanol/water partition

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*    coefficient (Kow). SARs have been used by the U.S. Environmental
*    Protection Agency since 1981 to predict the aquatic toxicity of new
*    industrial chemicals in the absence of test data.  SARs are developed for
*    chemical classes based on measured test data that have been submitted by
*    industry or they are developed by other sources for chemicals with
*    similar structures, e.g., phenols.  Using the measured aquatic toxicity
*    values and estimated Kow values, regression equations can be developed
*    for a class of chemicals.  Toxicity values for new chemicals may then be
*    calculated by inserting the estimated Kow into the regression equation
*    and correcting the resultant value for the molecular weight of the
*    compound.
**
**   To date, over 150 SARs have been developed for more than 50 chemical
*    classes.  These chemical classes range from the very large, e.g., neutral
*    organics, to the very small, e.g., aromatic diazoniums.  Some chemical
*    classes have only one SAR, such as acid chlorides, for which only a fish
*    96-hour LC50 has been developed.  The class with the greatest number of
*    SARs is the neutral organics, which has SARs ranging from acute and
*    chronic SARs for fish to a 14-day LC50 for earthworms in artificial soil.
*     The ECOSAR Class Program is a computerized version of the ECOSAR
*    analysis procedures as currently practiced by the Office of Pollution
*    Prevention and Toxics (OPPT).  It has been developed within the
*    regulatory constraints of the Toxic Substances Control Act (TSCA).  It is
*    a pragmatic approach to SAR as opposed to a theoretical approach.
F020 241201
EOR
F002 455
F010 4.1
F004 2
F005 RE
F006 ECOSAR v0.99h in EPI Suite (2000). Estimation Program Interface Suite,
*    v3.12.  Syracuse Research Corporation, Syracuse, NY, USA.
F007 ECOSAR v0.99h in EPI Suite (2000). Estimation Program Interface Suite,
*    v3.12.  Syracuse Research Corporation, Syracuse, NY, USA.
F020 241206
EOR
F002 455
F010 4.1
F004 2
F005 RL
F006 This robust summary has a reliability rating of 2 because the data are
*    calculated and not measured.
F007 This robust summary has a reliability rating of 2 because the data are
*    calculated and not measured.
F020 241205
EOR
F002 455
F010 4.1
F004 2
F005 RS
F006 LC50, 96 h, for fish = 214.1 mg/L
F007 LC50, 96 h, for fish = 214.1 mg/L
F020 241203
EOR
F002 455
F010 4.1
F004 2
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F005 TC
F006 Experimental water solubility, 8800 mg/l @ 20°C (Heitmann, W et al,
*   1987), log Kow, 1.52 (Funasaki, N et al, 1985) and melting point, -86.6°C
*   (SRC PhysProp database) were entered into the program.
**   Class: Neutral organics
F007 Experimental water solubility, 8800 mg/l @ 20°C (Heitmann, W et al,
*   1987), log Kow, 1.52 (Funasaki, N et al, 1985) and melting point, -86.6°C
*   (SRC PhysProp database) were entered into the program.
**   Class: Neutral organics
F020 241202
EOR
F002 455
F010 4.1
F004 2
F005 TS
F006 Diisopropyl Ether (CAS No. 108-20-3)
F007 Diisopropyl Ether (CAS No. 108-20-3)
F020 241214
EOR
F002 455
F010 4.1
F004 3
F005 CL
F006 96-hour LC50 = 786 mg/L based on mean measured values.
**   96-hour EC50 = 476 mg/L based on mean measured values.
F007 96-hour LC50 = 786 mg/L based on mean measured values.
**   96-hour EC50 = 476 mg/L based on mean measured values.
F020 243473
EOR
F002 455
F010 4.1
F004 3
F005 ME
F006 Test solutions were prepared using a proportional diluter system without
*   replication. This system provided control and five test substance
*   concentrations to glass test vessels. Each vessel held 2 L of test
*   solution and the diluter flow ra
F007 Test solutions were prepared using a proportional diluter system without
*   replication. This system provided control and five test substance
*   concentrations to glass test vessels. Each vessel held 2 L of test
*   solution and the diluter flow rate was sufficient to provide 18 volume
*   additions per day. An aqueous stock solution of 1050 mg/L was used by
*   the diluter to prepare the exposure series. Dilution water was filtered
*   Lake Superior water. Typical ranges of water quality factors measured in
*   this water were pH (7.4 - 8.2), total hardness (44 - 53 mg/L as CaCO3),
*   and specific conductance (78 - 86 mmhos/cm).
**
**   Test fish originated from in-house cultures of P. promelas at the U.S.
*   EPA Environmental Research Laboratory - Duluth. Fish were not fed 24 h
*   prior to testing or during the test. At test initiation, fish were
*   randomly placed in test vessels until each vessel contained 10
*   individuals. Individuals used in testing were 34 d old and measured 19.0
*   mm mean length (SD = 2.534) and 0.104 g mean weight (SD = 0.0433).
*   Biomass loading was 1.04 g/L. Death was the major test endpoint.
*   Numbers of dead fish were counted daily and any dead fish were removed
*   from the vessels. Abnormal behavioral changes were recorded at each
*   observation time. LC50 (lethality) and EC50 (total effect) values were

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*    determined.
**
**   Temperature, dissolved oxygen, and pH were measured daily in all test
*    chambers.  Mean values (and Standard Deviation) were 24.9 °C (SD = 0.52),
*    7.3 mg/L (SD = 0.13), and 7.75 (SD = 0.16), respectively.  Total hardness
*    and alkalinity were measured once in the control, low, medium, and high
*    test levels.  Mean values were 43.7 mg/L total hardness as CaCO3 (SD =
*    0.96) and 49.6 mg/L alkalinity as CaCO3 (SD = 0.25).  Lighting was
*    provided by fluorescent bulbs that produced 28 to 48 lumens/sq ft at the
*    water surface.  The photoperiod was 16 h light and 8 h dark.
**
**   Test substance concentrations were verified in most cases daily during
*    the test using gas-liquid chromatography.  Concentrations were averaged
*    and a mean percent recovery was calculated.  The nominal with measured
*    concentrations in parentheses were, control (not detected), 157 mg/L (131
*    mg/L), 242 mg/L (210 mg/L), 373 mg/L (382 mg/L), 574 mg/L (594 mg/L), and
*    883 mg/L (1044 mg/L).  The overall percent recovery was 98.7%.
F020 243470
EOR
F002 455
F010 4.1
F004 3
F005 RE
F006 Geiger D, Poirier S, Brooke L and Call D (eds.) (1986). Acute Toxicities
*    of Organic Chemicals to Fathead Minnows (Pimephales promelas), Vol. 3.
*    Center for Lake Superior Environmental Studies, Univ. of Wisconsin-
*    Superior, Superior, WI, USA.
F007 Geiger D, Poirier S, Brooke L and Call D (eds.) (1986). Acute Toxicities
*    of Organic Chemicals to Fathead Minnows (Pimephales promelas), Vol. 3.
*    Center for Lake Superior Environmental Studies, Univ. of Wisconsin-
*    Superior, Superior, WI, USA.
F020 243474
EOR
F002 455
F010 4.1
F004 3
F005 RM
F006 Statistics:  LC/EC50 values determined by Trimmed Spearman-Karber Method
F007 Statistics:  LC/EC50 values determined by Trimmed Spearman-Karber Method
F020 243471
EOR
F002 455
F010 4.1
F004 3
F005 RS
F006 96-hour LC50 = 786 mg/L based on mean measured values.
**   96-hour EC50 = 476 mg/L based on mean measured values.
**
**   The EC50 value was based on mortality and the following abnormal effects:
*    loss of schooling behavior, swimming near the surface,
F007 96-hour LC50 = 786 mg/L based on mean measured values.
**   96-hour EC50 = 476 mg/L based on mean measured values.
**
**   The EC50 value was based on mortality and the following abnormal effects:
*    loss of schooling behavior, swimming near the surface, hypoactive,
*    under-reactive to external stimuli, loss of equilibrium.
F020 243472
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EOR
F002 455
F010 4.1
F004 4
F005 CL
F006 96-h LC50 = 900 mg/L based on measured concentrations
F007 96-h LC50 = 900 mg/L based on measured concentrations
F020 243478
EOR
F002 455
F010 4.1
F004 4
F005 ME
F006 Test solutions were prepared using a continuous-flow diluter delivery
* system, which delivered four test substance concentrations and control
* solutions to duplicate test vessels. Dilution water was filtered Lake
* Superior water. Average val
F007 Test solutions were prepared using a continuous-flow diluter delivery
* system, which delivered four test substance concentrations and control
* solutions to duplicate test vessels. Dilution water was filtered Lake
* Superior water. Average values for water quality factors for the
* dilution water were: hardness (44.6 mg/L as CaCO3), total alkalinity
* (44.0 mg/L as CaCO3), and pH (7.6). Test chambers were glass vessels and
* contained 2 L of test solution. Solution flow rates through the test
* chambers was sufficient to provided at least a 95% replacement in
* approximately 4 h. Test substance concentrations were verified daily
* during the test using either gas chromatography or high pressure liquid
* chromatography methods.
**
** The mean temperature for the test was 25 ± 0.5°C, and dissolved oxygen
* remained at or above 80% saturation. Lighting was provided by wide
* spectrum fluorescent bulbs at an intensity of 22 to 38 lumens/sq ft over
* the test chambers. The photoperiod was 16 h light and 8 h dark with a
* 30-min dusk/dawn transition period.
**
** Test fish originated from cultures maintained by the U.S. EPA
* Environmental Research Laboratory - Duluth, MN. and were 28 to 34 days
* old (weighing approximately 0.12 g) at the time of testing. A total of
* 20 fish per treatment (10/replicate) was used in the test. Fish were
* added to the test chambers 2-3 h before introduction of the test
* solutions. Fish were not fed 24 h before or during the test.
* Mortalities were recorded daily.
F020 243475
EOR
F002 455
F010 4.1
F004 4
F005 RE
F006 Broderius S, and Kahl M (1985). Acute toxicity of organic chemical
* mixtures to the fathead minnow. Aquat. Toxicol. 6:307-322.
F007 Broderius S, and Kahl M (1985). Acute toxicity of organic chemical
* mixtures to the fathead minnow. Aquat. Toxicol. 6:307-322.
F020 243479
EOR
F002 455
F010 4.1
F004 4

F005 RM
F006 Statistics: Trimmed Spearman-Karber Method or log-probit method.
F007 Statistics: Trimmed Spearman-Karber Method or log-probit method.
F020 243476
EOR
F002 455
F010 4.1
F004 4
F005 RS
F006 96-h LC50 = 900 mg/L based on measured concentrations
**   95% CL = 881 - 920 mg/L
F007 96-h LC50 = 900 mg/L based on measured concentrations
**   95% CL = 881 - 920 mg/L
F020 243477
EOR
F002 455
F010 4.1
F004 5
F005 CL
F006 24-hour LC50 = 380 mg/L.
F007 24-hour LC50 = 380 mg/L.
F020 243483
EOR
F002 455
F010 4.1
F004 5
F005 ME
F006 The test consisted of exposing groups of six fish to a series of
*   concentrations of the test substance for 24 h. Fish were exposed in an
*   all glass tanks holding 25 liters of test solution. Dilution water was
*   local tap water having the foll
F007 The test consisted of exposing groups of six fish to a series of
*   concentrations of the test substance for 24 h. Fish were exposed in an
*   all glass tanks holding 25 liters of test solution. Dilution water was
*   local tap water having the following characteristics (all values in mg/L):
** Cl^{-} = 65; $NO2^{-}$ = 0; $NO3^{-}$ = 4; $SO4^{-}2$ = 35; $PO4^{-}3$ = 0.15; $HCO3^{-}$ = 25; SiO2
*   = 25; NH4+ = 0; Fe = 0.05; Mn = 0; Ca+2 = 100; Mg+2 = 8; alkali as Na+ =
*   30; pH = 7.8.
**
**   The test was run at a temperature of 20±1°C, and the solutions were not
*   aerated during the test period.
**
**   Test fish had a mean length of 6.2±0.7 cm, a mean weight of 3.3 ± 1.0 g
*   and were in good health at the time of testing.
**
**   Exposure concentrations were confirmed either by total organic carbon
*   analysis or by extraction and subsequent analysis by gas chromatography.
*   Measured concentrations were not reported in this study.
F020 243480
EOR
F002 455
F010 4.1
F004 5
F005 RE
F006 Bridie A, Wolff C and Winter M (1979). The acute toxicity of some
*   petrochemicals to goldfish. Water Res. 13:623-626.
F007 Bridie A, Wolff C and Winter M (1979). The acute toxicity of some

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*    petrochemicals to goldfish. Water Res. 13:623-626.
F020 243485
EOR
F002 455
F010 4.1
F004 5
F005 RL
F006 The test was run for only 24 hours to ensure that the dissolved oxygen
*    content did not fall below 4 mg/L. The report lacked sufficient detail
*    for assessment.  It was not stated whether results were based on nominal
*    or measured values.
F007 The test was run for only 24 hours to ensure that the dissolved oxygen
*    content did not fall below 4 mg/L. The report lacked sufficient detail
*    for assessment.  It was not stated whether results were based on nominal
*    or measured values.
F020 243484
EOR
F002 455
F010 4.1
F004 5
F005 RM
F006 Determination of LC50 by graphical interpolation of log concentrations
*    versus percent mortality (APHA, 1971).
F007 Determination of LC50 by graphical interpolation of log concentrations
*    versus percent mortality (APHA, 1971).
F020 243481
EOR
F002 455
F010 4.1
F004 5
F005 RS
F006 24-hour LC50 = 380 mg/L
**
**   The analytical method was either total organic carbon analysis or gas
*    chromatography.  It was not reported what method was employed for this
*    test substance nor if the result was based on measured concentrations.
F007 24-hour LC50 = 380 mg/L
**
**   The analytical method was either total organic carbon analysis or gas
*    chromatography.  It was not reported what method was employed for this
*    test substance nor if the result was based on measured concentrations.
F020 243482
EOR
F002 455
F010 4.1
F004 6
F005 CL
F006 96-hour LC50 = 7,000 mg/L based on nominal concentrations
F007 96-hour LC50 = 7,000 mg/L based on nominal concentrations
F020 243489
EOR
F002 455
F010 4.1
F004 6
F005 ME
F006 The test consisted of exposing groups of fish to a four-dilution series
*    of the test substance for a period of 96 h.  Test vessels were all glass
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*    5-gallon aquaria.  The volume of test solution was adjusted to assure
*    that a biomass loading wa
F007 The test consisted of exposing groups of fish to a four-dilution series
*    of the test substance for a period of 96 h.  Test vessels were all glass
*    5-gallon aquaria.  The volume of test solution was adjusted to assure
*    that a biomass loading was no more than 1 g fish /liter solution.
*    Dilution water was well water having a typical pH of 7.6 to 7.9 and a
*    hardness of 55 mg/L (as CaCO3).
**
**   Fish were obtained from a commercial source and assessed for health
*    during a 14-d acclimation period prior to testing. During that time they
*    were maintained on a commercial fish food diet supplemented with minced
*    frozen shrimp. Fish were not fed 48 hours prior to testing.  Fish were
*    randomly selected for testing and were approximately 33 to 75 mm in
*    length.
**
**   The test was run at 23°C.  Test solutions were not aerated for the
*    initial 24 h, but aeration was applied thereafter if the dissolved oxygen
*    concentration was being depleted.  Dissolved oxygen readings were taken
*    daily, and pH was measured at the end of the test. However, these data
*    were not provided in the report.
**
**   Mortality was assessed daily and any dead fish were removed at each
*    observation time.
F020 243486
EOR
F002 455
F010 4.1
F004 6
F005 RE
F006 Dawson G, Jennings A, Drozdowski D and Rider E (1975/77). The acute
*    toxicity of 47 industrial chemicals to fresh and saltwater fishes. J.
*    Haz. Mat. 1:303-318.
F007 Dawson G, Jennings A, Drozdowski D and Rider E (1975/77). The acute
*    toxicity of 47 industrial chemicals to fresh and saltwater fishes. J.
*    Haz. Mat. 1:303-318.
F020 243491
EOR
F002 455
F010 4.1
F004 6
F005 RL
F006 Documentation was insufficient for evaluation. Basic water quality data
*    during the test were not provided.  The authors stated that aeration of
*    the test solutions was used after 24 hours to ensure maintenance of
*    dissolved oxygen.  No analyt
F007 Documentation was insufficient for evaluation. Basic water quality data
*    during the test were not provided.  The authors stated that aeration of
*    the test solutions was used after 24 hours to ensure maintenance of
*    dissolved oxygen.  No analytical verification of exposure concentrations
*    were made.
F020 243490
EOR
F002 455
F010 4.1
F004 6
F005 RM
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F006 The LC50 was determined by plotting survival percentages on
*   semi-logarithmic paper and drawing a straight line fit through or near
*   significant points above and below 50% survival.
F007 The LC50 was determined by plotting survival percentages on
*   semi-logarithmic paper and drawing a straight line fit through or near
*   significant points above and below 50% survival.
F020 243487
EOR
F002 455
F010 4.1
F004 6
F005 RS
F006 96-hour LC50 = 7,000 mg/L
**
**   The mortality pattern reported for the test substance suggests that a
*   more likely estimate of the LC50 value would lie between 7,900 and 10,000
*   mg/L, rather than 7,000 mg/L. This was due to a non-monotonic dose re
F007 96-hour LC50 = 7,000 mg/L
**
**   The mortality pattern reported for the test substance suggests that a
*   more likely estimate of the LC50 value would lie between 7,900 and 10,000
*   mg/L, rather than 7,000 mg/L. This was due to a non-monotonic dose
*   response pattern of mortality. The report authors indicated that the LC50
*   value was higher than the published solubility for the test substance.
F020 243488
EOR
F002 455
F010 4.1
F004 7
F005 CL
F006 96-hour LC50 = 6600 mg/L based on nominal concentrations.
F007 96-hour LC50 = 6600 mg/L based on nominal concentrations.
F020 243495
EOR
F002 455
F010 4.1
F004 7
F005 ME
F006 The test consisted of exposing groups of fish to a four-dilution series
*   of the test substance for a period of 96 h. Test vessels were all glass
*   5-gallon aquaria. The volume of test solution was adjusted to assure
*   that a biomass loading wa
F007 The test consisted of exposing groups of fish to a four-dilution series
*   of the test substance for a period of 96 h. Test vessels were all glass
*   5-gallon aquaria. The volume of test solution was adjusted to assure
*   that a biomass loading was no more than 1 g fish /liter solution.
*   Dilution water was prepared by adding "instant ocean" salts to well water
*   (pH of 7.6 to 7.9; hardness 55 mg/L (as CaCO3)) until a specific gravity
*   of 1.018 was achieved.
**
**   Fish were field collected in nets from Horseshoe Bay at Sandy Hook, New
*   Jersey. They were held for a 14-d acclimation period prior to testing and
*   assessed for health during that time. During the acclimation period they
*   were fed minced frozen shrimp. Fish were not fed 48 hours prior to
*   testing. Fish were randomly selected for testing and were approximately
*   40 to 100 mm in length.
**

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**   The test was run at 20°C, and test solutions were continuously aerated
*    during the exposure period. Dissolved oxygen readings were taken daily,
*    and pH was measured at the end of the test. However, these data were not
*    provided in the report.
**
**   Mortality was assessed daily and any dead fish were removed at each
*    observation time.
F020 243492
EOR
F002 455
F010 4.1
F004 7
F005 RE
F006 Dawson G, Jennings A, Drozdowski D and Rider E (1975/77). The acute
*    toxicity of 47 industrial chemicals to fresh and saltwater fishes. J.
*    Haz. Mat. 1:303-318.
F007 Dawson G, Jennings A, Drozdowski D and Rider E (1975/77). The acute
*    toxicity of 47 industrial chemicals to fresh and saltwater fishes. J.
*    Haz. Mat. 1:303-318.
F020 243497
EOR
F002 455
F010 4.1
F004 7
F005 RL
F006 Documentation was insufficient for evaluation. Basic water quality data
*    during the test were not provided.  The authors stated that aeration of
*    the test solutions was used after 24 hours to ensure maintenance of
*    dissolved oxygen.  No analyt
F007 Documentation was insufficient for evaluation. Basic water quality data
*    during the test were not provided.  The authors stated that aeration of
*    the test solutions was used after 24 hours to ensure maintenance of
*    dissolved oxygen.  No analytical verification of exposure concentrations
*    were made.
F020 243496
EOR
F002 455
F010 4.1
F004 7
F005 RM
F006 LC50 determined by graphical interpolation of the logarithm of the
*    concentration versus the percentage mortality.
F007 LC50 determined by graphical interpolation of the logarithm of the
*    concentration versus the percentage mortality.
F020 243493
EOR
F002 455
F010 4.1
F004 7
F005 RS
F006 96-hour LC50 = 6600 mg/L
**
**   The mortality pattern reported for the test substance does not correspond
*    with the estimated LC50 value.  Given the dose-response pattern, the LC50
*    value would lie between 3,200 and 5,000 mg/L, rather than 6,600 mg
F007 96-hour LC50 = 6600 mg/L
**
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** The mortality pattern reported for the test substance does not correspond
* with the estimated LC50 value. Given the dose-response pattern, the LC50
* value would lie between 3,200 and 5,000 mg/L, rather than 6,600 mg/L.
* The authors reported that the result was higher than the reported water
* solubility of the test substance.
F020 243494
EOR
F002 455
F010 4.2
F004 1
F005 CL
F006 After Daphnia magna were exposed to test solutions of di-isopropyl ether
* for 48 hours in a static test, the 24 h and 48 h EC50 values were
* calculated to be 240 mg/L and 190 mg/L, respectively.
F007 After Daphnia magna were exposed to test solutions of di-isopropyl ether
* for 48 hours in a static test, the 24 h and 48 h EC50 values were
* calculated to be 240 mg/L and 190 mg/L, respectively.
F020 241346
EOR
F002 455
F010 4.2
F004 1
F005 RE
F006 Stephenson R (1983). Isopropyl Ether: Acute Toxicity to Daphnia magna and
* Selenastrum capricornutum. Group Research Limited, Report No.
* SBGR.83.215. Shell Research Ltd. Sittingbourne Research Centre,
* Sittingbourne, UK.
F007 Stephenson R (1983). Isopropyl Ether: Acute Toxicity to Daphnia magna and
* Selenastrum capricornutum. Group Research Limited, Report No.
* SBGR.83.215. Shell Research Ltd. Sittingbourne Research Centre,
* Sittingbourne, UK.
F008 HEDSET
F009 19-10-1993
F020 235981
EOR
F002 455
F010 4.2
F004 1
F005 RL
F006 This robust summary has a reliability rating of 2 because it did not
* analytically verify exposure concentrations and the results are based on
* nominal values.
F007 This robust summary has a reliability rating of 2 because it did not
* analytically verify exposure concentrations and the results are based on
* nominal values.
F020 241348
EOR
F002 455
F010 4.2
F004 1
F005 RM
F006 Statistics:
** Probit analysis after log transformation of the concentrations (Finney,
* 1971)
** Probit Analysis, Finney, D.J., Cambridge University Press, 3rd edition,
* p333 (1971)
F007 Statistics:

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**   Probit analysis after log transformation of the concentrations (Finney,
*    1971)
**   Probit Analysis, Finney, D.J., Cambridge University Press, 3rd edition,
*    p333 (1971)
F020 241349
EOR
F002 455
F010 4.2
F004 1
F005 RS
F006 The 24 h and 48 h Effect Concentration (EC50) values were calculated to
*    be 240 mg/L (95% fiducial limits 210 to 280 mg/L) and 190 mg/L (95%
*    fiducial limits 160 to 220 mg/L), respectively.
**   The immobilization (%) of Daphnia magna (n=10/replic
F007 The 24 h and 48 h Effect Concentration (EC50) values were calculated to
*    be 240 mg/L (95% fiducial limits 210 to 280 mg/L) and 190 mg/L (95%
*    fiducial limits 160 to 220 mg/L), respectively.
**   The immobilization (%) of Daphnia magna (n=10/replicate) are as follows:
**
**   Test Substance       Immobilization (%)*
**     Loading Rate
**          (mg/L)          24 hr     48 hr
**
**      0 (control)          0         0
**           46              0         0
**           99              3         7
**          210             27        57
**          460            100       100
**         1000            100       100
**   *mean of 3 replicates
F020 241345
EOR
F002 455
F010 4.2
F004 1
F005 TC
F006 A 48 hour static toxicity test was carried out without renewal of the
*    test solutions. Quantities of stock solutions of di-isopropyl ether in
*    acetone were added in triplicate sets of 110 mL glass flasks so that when
*    made up with reconstitute
F007 A 48 hour static toxicity test was carried out without renewal of the
*    test solutions. Quantities of stock solutions of di-isopropyl ether in
*    acetone were added in triplicate sets of 110 mL glass flasks so that when
*    made up with reconstituted freshwater, an approximately logarithmic
*    series of concentrations ranging from 46 to 1000 mg/L was produced. Three
*    flasks served as controls and received no test substance. The
*    concentration of acetone in all control and test flasks was 0.1 mL/L.
*    Precautions were taken to (a) minimise evaporative loss of the test
*    substance by use of glass cover slips over the vessel necks and (b) to
*    minimize the risk of organisms becoming trapped at the surface by placing
*    black paper caps over the flasks to create a darkened zone which the
*    organisms would avoid.
**   The test temperatures were in the range 20 ± 2°C, pH was in the range 8.2
*    to 8.4, the total hardness was 164 mg/L as CaCO3, and dissolved oxygen
*    was in the range 8.2 to 9.2 mg/L.
**   The daphnids were cultured in-house, derived from a strain obtained (via
*    ICI Brixham Laboratory) from Institut National de Recherche Chimique
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*    Applique (I.R.Ch.A.), France. Age was <24 hours old from 15 to 35 day old
*    parents.
**   All concentrations of test substance are expressed in terms of quantities
*    initially added to the test vessels.
F020 241344
EOR
F002 455
F010 4.2
F004 1
F005 TS
F006 Diisopropyl Ether (CAS No. 108-20-3)
F007 Diisopropyl Ether (CAS No. 108-20-3)
F020 241347
EOR
F002 455
F010 4.2
F004 2
F005 CL
F006 The predicted 48 h LC50 value for Daphnia (221.9 mg/L) is in close
*    agreement with the experimental 48 h EC50 value for Daphnia (190.0 mg/L)
*    (Stephenson R.R., Shell Research Limited, Report No. SBGR.83.215).
F007 The predicted 48 h LC50 value for Daphnia (221.9 mg/L) is in close
*    agreement with the experimental 48 h EC50 value for Daphnia (190.0 mg/L)
*    (Stephenson R.R., Shell Research Limited, Report No. SBGR.83.215).
F020 241211
EOR
F002 455
F010 4.2
F004 2
F005 ME
F006 ECOSAR version 0.99h, US EPA. The structure-activity relationships (SARs)
*    presented in this program are used to predict the aquatic toxicity of
*    chemicals based on their similarity of structure to chemicals for which
*    the aquatic toxicity has
F007 ECOSAR version 0.99h, US EPA. The structure-activity relationships (SARs)
*    presented in this program are used to predict the aquatic toxicity of
*    chemicals based on their similarity of structure to chemicals for which
*    the aquatic toxicity has been previously measured.  Most SAR calculations
*    in the ECOSAR Class Program are based upon the octanol/water partition
*    coefficient (Kow). SARs have been used by the U.S. Environmental
*    Protection Agency since 1981 to predict the aquatic toxicity of new
*    industrial chemicals in the absence of test data.  SARs are developed for
*    chemical classes based on measured test data that have been submitted by
*    industry or they are developed by other sources for chemicals with
*    similar structures, e.g., phenols.  Using the measured aquatic toxicity
*    values and estimated Kow values, regression equations can be developed
*    for a class of chemicals.  Toxicity values for new chemicals may then be
*    calculated by inserting the estimated Kow into the regression equation
*    and correcting the resultant value for the molecular weight of the
*    compound.
**
**   To date, over 150 SARs have been developed for more than 50 chemical
*    classes.  These chemical classes range from the very large, e.g., neutral
*    organics, to the very small, e.g., aromatic diazoniums.  Some chemical
*    classes have only one SAR, such as acid chlorides, for which only a fish
*    96-hour LC50 has been developed.  The class with the greatest number of
*    SARs is the neutral organics, which has SARs ranging from acute and
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*    chronic SARs for fish to a 14-day LC50 for earthworms in artificial soil.
*     The ECOSAR Class Program is a computerized version of the ECOSAR
*    analysis procedures as currently practiced by the Office of Pollution
*    Prevention and Toxics (OPPT).  It has been developed within the
*    regulatory constraints of the Toxic Substances Control Act (TSCA).  It is
*    a pragmatic approach to SAR as opposed to a theoretical approach.
F020 241207
EOR
F002 455
F010 4.2
F004 2
F005 RE
F006 ECOSAR v0.99h in EPI Suite (2000). Estimation Program Interface Suite,
*    v3.12.  Syracuse Research Corporation, Syracuse, NY, USA.
F007 ECOSAR v0.99h in EPI Suite (2000). Estimation Program Interface Suite,
*    v3.12.  Syracuse Research Corporation, Syracuse, NY, USA.
F020 241213
EOR
F002 455
F010 4.2
F004 2
F005 RL
F006 This robust summary has a reliability rating of 2 because the data are
*    calculated and not measured.
F007 This robust summary has a reliability rating of 2 because the data are
*    calculated and not measured.
F020 241212
EOR
F002 455
F010 4.2
F004 2
F005 RS
F006 EC50, 48 h, for Daphnia = 221.9 mg/L
F007 EC50, 48 h, for Daphnia = 221.9 mg/L
F020 241209
EOR
F002 455
F010 4.2
F004 2
F005 TC
F006 Experimental water solubility, 8800 mg/l @ 20°C (Heitmann, W et al,
*    1987), log Kow, 1.52 (Funasaki, N et al, 1985) and melting point, -86.6°C
*    (SRC PhysProp database) were entered into the program.
**   Class: Neutral organics
F007 Experimental water solubility, 8800 mg/l @ 20°C (Heitmann, W et al,
*    1987), log Kow, 1.52 (Funasaki, N et al, 1985) and melting point, -86.6°C
*    (SRC PhysProp database) were entered into the program.
**   Class: Neutral organics
F020 241208
EOR
F002 455
F010 4.2
F004 2
F005 TS
F006 Diisopropyl Ether, CAS No. 108-20-3
F007 Diisopropyl Ether, CAS No. 108-20-3
F020 241210
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EOR
F002 455
F010 4.3
F004 2
F005 CL
F006 The predicted 96 h EC50 value for algae (134.9 mg/L) is in the same range
*   as the predicted 48 h LC50 value for Daphnia (221.9 mg/L) and the
*   predicted 96 h LC50 value for fish (214.1 mg/L). There is also good
*   comparison between the predicted
F007 The predicted 96 h EC50 value for algae (134.9 mg/L) is in the same range
*   as the predicted 48 h LC50 value for Daphnia (221.9 mg/L) and the
*   predicted 96 h LC50 value for fish (214.1 mg/L). There is also good
*   comparison between the predicted and experimental EC50 values for Daphnia
*   (221.9 mg/l v 190.0 mg/L, respectively) and for fish (214.1 mg/l v 91.7
*   mg/L, respectively).
F020 241198
EOR
F002 455
F010 4.3
F004 2
F005 ME
F006 ECOSAR version 0.99h, US EPA. The structure-activity relationships (SARs)
*   presented in this program are used to predict the aquatic toxicity of
*   chemicals based on their similarity of structure to chemicals for which
*   the aquatic toxicity has
F007 ECOSAR version 0.99h, US EPA. The structure-activity relationships (SARs)
*   presented in this program are used to predict the aquatic toxicity of
*   chemicals based on their similarity of structure to chemicals for which
*   the aquatic toxicity has been previously measured. Most SAR calculations
*   in the ECOSAR Class Program are based upon the octanol/water partition
*   coefficient (Kow). SARs have been used by the U.S. Environmental
*   Protection Agency since 1981 to predict the aquatic toxicity of new
*   industrial chemicals in the absence of test data. SARs are developed for
*   chemical classes based on measured test data that have been submitted by
*   industry or they are developed by other sources for chemicals with
*   similar structures, e.g., phenols. Using the measured aquatic toxicity
*   values and estimated Kow values, regression equations can be developed
*   for a class of chemicals. Toxicity values for new chemicals may then be
*   calculated by inserting the estimated Kow into the regression equation
*   and correcting the resultant value for the molecular weight of the
*   compound.
**
**   To date, over 150 SARs have been developed for more than 50 chemical
*   classes. These chemical classes range from the very large, e.g., neutral
*   organics, to the very small, e.g., aromatic diazoniums. Some chemical
*   classes have only one SAR, such as acid chlorides, for which only a fish
*   96-hour LC50 has been developed. The class with the greatest number of
*   SARs is the neutral organics, which has SARs ranging from acute and
*   chronic SARs for fish to a 14-day LC50 for earthworms in artificial soil.
*   The ECOSAR Class Program is a computerized version of the ECOSAR
*   analysis procedures as currently practiced by the Office of Pollution
*   Prevention and Toxics (OPPT). It has been developed within the
*   regulatory constraints of the Toxic Substances Control Act (TSCA). It is
*   a pragmatic approach to SAR as opposed to a theoretical approach.
F020 241195
EOR
F002 455

F010 4.3
F004 2
F005 RE
F006 ECOSAR v0.99h in EPI Suite (2000). Estimation Program Interface Suite,
*   v3.12. Syracuse Research Corporation, Syracuse, NY, USA.
F007 ECOSAR v0.99h in EPI Suite (2000). Estimation Program Interface Suite,
*   v3.12. Syracuse Research Corporation, Syracuse, NY, USA.
F020 241200
EOR
F002 455
F010 4.3
F004 2
F005 RL
F006 This robust summary has a reliability rating of 2 because the data are
*   calculated and not measured.
F007 This robust summary has a reliability rating of 2 because the data are
*   calculated and not measured.
F020 241199
EOR
F002 455
F010 4.3
F004 2
F005 RS
F006 EC50, 96 h, for green algae = 134.9 mg/L
**
**   ChV, 96 h, for green algae = 10.2 mg/L
F007 EC50, 96 h, for green algae = 134.9 mg/L
**
**   ChV, 96 h, for green algae = 10.2 mg/L
F020 241197
EOR
F002 455
F010 4.3
F004 2
F005 TC
F006 Experimental water solubility, 8800 mg/l @ 20°C (Heitmann, W et al,
*   1987), log Kow, 1.52 (Funasaki, N et al, 1985) and melting point, -86.6°C
*   (SRC PhysProp database) were entered into the program.
**   Class: Neutral organics
F007 Experimental water solubility, 8800 mg/l @ 20°C (Heitmann, W et al,
*   1987), log Kow, 1.52 (Funasaki, N et al, 1985) and melting point, -86.6°C
*   (SRC PhysProp database) were entered into the program.
**   Class: Neutral organics
F020 241196
EOR
F002 455
F010 4.3
F004 2
F005 TS
F006 Diisopropyl Ether (CAS No. 108-20-3)
F007 Diisopropyl Ether (CAS No. 108-20-3)
F020 241215
EOR
F002 455
F010 4.3
F004 3
F005 CL

F006 96-hour EC50 = >1000 mg/L based on nominal concentrations.
F007 96-hour EC50 = >1000 mg/L based on nominal concentrations.
F020 243500
EOR
F002 455
F010 4.3
F004 3
F005 ME
F006 A 4 d algal growth study was carried out using 10 concentrations of the
* test substance and a control. The test design included six control
* replicates and single vessels dosed with different concentrations of the
* test substance. 250-mL gla
F007 A 4 d algal growth study was carried out using 10 concentrations of the
* test substance and a control. The test design included six control
* replicates and single vessels dosed with different concentrations of the
* test substance. 250-mL glass Erlenmeyer flasks served as the test
* vessels and held 50 mL of culture medium. Culture medium was prepare
* following the recipe given by Miller and Green (1978) with the following
* exceptions; 1) boric acid concentration = 105 mg/L, and 2) sodium
* bicarbonate concentration = 50 mg/L.
**
** To 10 flasks, quantities of a test substance stock solution made up in
* acetone were added to give a logarithmic series of concentrations ranging
* from 1 to 1000 mg/L (1.0, 2.2, 4.6, 10, 22, 46, 100, 220, 460, and 1000
* mg/L). The concentration of acetone in all flasks including controls was
* adjusted to 0.1 mL/L. Each flask was inoculated with S. capricornutum to
* give an initial cell density of 5 x 102 cells/mL. The algal inoculum was
* prepared from an actively growing liquid culture of S. capricornutum in
* exponential growth phase.
**
** Flasks were incubated in a temperature controlled orbital incubator under
* constant illumination (approximately 3000 lux) at 24±2°C for 4 days.
* Cell counts were made on days 2 and 4 using an electronic particle
* counter (Coulter counter). The temperature in the incubator was measured
* at 4-h intervals. The pH of the control and highest test concentration
* was measured on days 0, 2, and 4. Temperature remained within the 24±2°C
* specified range, and the pH ranged from 8.3 to 8.5 in the measured
* vessels.
**
** All determination of EC50 values were based on nominal test
* concentrations and cell counts.
F020 243498
EOR
F002 455
F010 4.3
F004 3
F005 RE
F006 Stephenson R (1983). Isopropyl ether: Acute toxicity to Daphnia magna and
* Selenastrum capricornutum. Report # SBGR.83.215, Shell Research Ltd.
* Sittingbourne Research Centre, Sittingbourne, Kent, England.
F007 Stephenson R (1983). Isopropyl ether: Acute toxicity to Daphnia magna and
* Selenastrum capricornutum. Report # SBGR.83.215, Shell Research Ltd.
* Sittingbourne Research Centre, Sittingbourne, Kent, England.
F020 243502
EOR
F002 455
F010 4.3

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F004 3
F005 RL
F006 Test concentrations were not measured and there is no indication in the
*    report whether the test vessels were sealed. The reported LC50 value may
*    reflect a loss of test substance by volatilization if the flasks were not
*    tightly sealed.
F007 Test concentrations were not measured and there is no indication in the
*    report whether the test vessels were sealed. The reported LC50 value may
*    reflect a loss of test substance by volatilization if the flasks were not
*    tightly sealed.
F020 243501
EOR
F002 455
F010 4.3
F004 3
F005 RS
F006 96-hour EC50 = >1000 mg/L based on nominal concentrations.
**
**   The 96-hour cell counts in the treated flasks as a percent of the mean
*    control cell counts were:
**    1.0 mg/L = 84%     46 mg/L = 127%
**    2.2 mg/L = 108%   100 mg/L = 130%
**    4.6 mg/L = 91%    22
F007 96-hour EC50 = >1000 mg/L based on nominal concentrations.
**
**   The 96-hour cell counts in the treated flasks as a percent of the mean
*    control cell counts were:
**    1.0 mg/L = 84%     46 mg/L = 127%
**    2.2 mg/L = 108%   100 mg/L = 130%
**    4.6 mg/L = 91%    220 mg/L = 113%
**    10 mg/L = 122%    460 mg/L = 127%
**    22 mg/L = 129%    1000 mg/L = 91%
F020 243499
EOR
F002 455
F010 5.1.1
F004 5
F005 CL
F006 DIPE, when administered to adult male Sprague-Dawley rats, had an acute
*    oral LD50 of >10 g/kg. 14-day immature rats were considerable more
*    sensitive [LD50  4.5 g/kg].
F007 DIPE, when administered to adult male Sprague-Dawley rats, had an acute
*    oral LD50 of >10 g/kg. 14-day immature rats were considerable more
*    sensitive [LD50  4.5 g/kg].
F020 241249
EOR
F002 455
F010 5.1.1
F004 5
F005 ME
F006 Administered orally to nonfasted rats. LD50 calculated by the method of
*    Litchfield and Wilcoxon [1949]. Similar to OECD 401.
F007 Administered orally to nonfasted rats. LD50 calculated by the method of
*    Litchfield and Wilcoxon [1949]. Similar to OECD 401.
F020 241245
EOR
F002 455
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F010 5.1.1
F004 5
F005 RE
F006 Kimura ET, Ebert DM and Doge PW (1971). Acute toxicity and limits of
*   solvent residues for sixteen organic solvents. Toxicol. Appl. Pharmacol.
*   19:699-704.
F007 Kimura ET, Ebert DM and Doge PW (1971). Acute toxicity and limits of
*   solvent residues for sixteen organic solvents. Toxicol. Appl. Pharmacol.
*   19:699-704.
F020 241250
EOR
F002 455
F010 5.1.1
F004 5
F005 RL
F006 Not GLP but conducted at a reputable laboratory [Abbot Laboratories,
*   Chicago].
F007 Not GLP but conducted at a reputable laboratory [Abbot Laboratories,
*   Chicago].
F020 241251
EOR
F002 455
F010 5.1.1
F004 5
F005 RM
F006 Test type: Acute oral toxicity
**   Year: Prior to 1971
**   No. of animals/dose: 6 male for young adult and older adult
**   6 - 12 male and female for 14-day old rats
**   Route of administration: Oral gavage
**   Dose level: Variable
**   Dose volume: Variable
F007 Test type: Acute oral toxicity
**   Year: Prior to 1971
**   No. of animals/dose: 6 male for young adult and older adult
**   6 - 12 male and female for 14-day old rats
**   Route of administration: Oral gavage
**   Dose level: Variable
**   Dose volume: Variable
**   Control group included: No, but none needed
F020 241248
EOR
F002 455
F010 5.1.1
F004 5
F005 RS
F006 14-day old: LD50 6.4 ml/kg [approx 4.5 g/kg]
**   young adults: LD50 16.5 ml/kg [approx 11.6 g/kg]
**   Older adults: LD50 16.0 ml/kg [approx 11.2 g/kg]
**
**   G/kg dose based on a density of 0.72 g/ml
F007 14-day old: LD50 6.4 ml/kg [approx 4.5 g/kg]
**   young adults: LD50 16.5 ml/kg [approx 11.6 g/kg]
**   Older adults: LD50 16.0 ml/kg [approx 11.2 g/kg]
**
**   G/kg dose based on a density of 0.72 g/ml
F020 241247

EOR
F002 455
F010 5.1.1
F004 5
F005 TC
F006 Rats were observed for up to 7 days after dosing.
F007 Rats were observed for up to 7 days after dosing.
F020 241246
EOR
F002 455
F010 5.1.1
F004 5
F005 TS
F006 Diisopropyl ether (CAS No. 108-20-3)
** Chemical name: Isopropyl ether; isopropoxy propane, 2-; oxybis
* [propane], 2,2 '-
** Source/purity of test material is not specified, but stated to be
* analytical grade meeting ACS specifications.
F007 Diisopropyl ether (CAS No. 108-20-3)
** Chemical name: Isopropyl ether; isopropoxy propane, 2-; oxybis
* [propane], 2,2 '-
** Source/purity of test material is not specified, but stated to be
* analytical grade meeting ACS specifications.
F020 241244
EOR
F002 455
F010 5.1.1
F004 6
F005 CL
F006 The test article, when administered orally as received to New Zealand
* white rabbits had a minimal lethal dose of 7 - 9 ml/kg [approx 5 - 6.5
* g/kg].
F007 The test article, when administered orally as received to New Zealand
* white rabbits had a minimal lethal dose of 7 - 9 ml/kg [approx 5 - 6.5
* g/kg].
F020 241254
EOR
F002 455
F010 5.1.1
F004 6
F005 RE
F006 Machle W, Scott EW and Treon J (1939). The physiological response to
* isopropyl ether and to a mixture of isopropyl ether and gasoline. J. Ind.
* Hyg. Toxicol. 21:72-96.
F007 Machle W, Scott EW and Treon J (1939). The physiological response to
* isopropyl ether and to a mixture of isopropyl ether and gasoline. J. Ind.
* Hyg. Toxicol. 21:72-96.
F020 241256
EOR
F002 455
F010 5.1.1
F004 6
F005 RL
F006 Not conducted by GLP but at a reputable laboratory [Kettering Laboratory,
* University of Cincinnati].
F007 Not conducted by GLP but at a reputable laboratory [Kettering Laboratory,
* University of Cincinnati].

F020 241255
EOR
F002 455
F010 5.1.1
F004 6
F005 RM
F006 Test type: Acute oral toxicity
**   Year: Prior to 1939
**   Route of administration: Oral
**   Dose levels: 8.2, 7.2, 6.0, 5.2, 3.3, 1.62 g/kg
**   Dose volume: Variable
**   Control: No - none needed
F007 Test type: Acute oral toxicity
**   Year: Prior to 1939
**   Route of administration: Oral
**   Dose levels: 8.2, 7.2, 6.0, 5.2, 3.3, 1.62 g/kg
**   Dose volume: Variable
**   Control: No - none needed
F020 241257
EOR
F002 455
F010 5.1.1
F004 6
F005 RS
F006 Minimal lethal dose between 7 - 9 ml/kg
**
**   The symptoms noted were lack of coordination and unsteadiness at onset
*   followed by a slight narcosis. In the animals that died the narcosis
*   progressed towards a deep narcosis with loss of corneal re
F007 Minimal lethal dose between 7 - 9 ml/kg
**
**   The symptoms noted were lack of coordination and unsteadiness at onset
*   followed by a slight narcosis. In the animals that died the narcosis
*   progressed towards a deep narcosis with loss of corneal reflex and
*   evidences of depressant action on the medulla appeared, respiration
*   became progressively slower, irregular and variable in amplitude and drop
*   in body temperature till respiration failed. In the surviving animals, no
*   effect on HB, erythrocyte count, total and differential leukocyte count
*   was observed. No delayed toxicity was observed during the recovery period
*   of 4 months after treatment.
F020 241253
EOR
F002 455
F010 5.1.1
F004 6
F005 TS
F006 Diisopropyl ether (CAS No. 108-20-3)
**   Chemical name: Isopropyl ether; isopropoxy propane, 2-; oxybis
*   [propane], 2,2 '-
**   Test material is stated to be commercial grade with 3% of isopropyl
*   alcohol, but with no peroxide nor added inhibitor.
F007 Diisopropyl ether (CAS No. 108-20-3)
**   Chemical name: Isopropyl ether; isopropoxy propane, 2-; oxybis
*   [propane], 2,2 '-
**   Test material is stated to be commercial grade with 3% of isopropyl
*   alcohol, but with no peroxide nor added inhibitor.
F020 241252

EOR
F002 455
F010 5.1.2
F004 2
F005 CL
F006 The lowest lethal dose for 1 hr exposure was greater than 30,000 ppm in
*   three species.
F007 The lowest lethal dose for 1 hr exposure was greater than 30,000 ppm in
*   three species.
F020 241267
EOR
F002 455
F010 5.1.2
F004 2
F005 RE
F006 Machle W, Scott EW and Treon J (1939). The physiological response to
*   isopropyl ether and to a mixture of isopropyl ether and gasoline. J. Ind.
*   Hyg. Toxicol. 21:72-96.
F007 Machle W, Scott EW and Treon J (1939). The physiological response to
*   isopropyl ether and to a mixture of isopropyl ether and gasoline. J. Ind.
*   Hyg. Toxicol. 21:72-96.
F020 241273
EOR
F002 455
F010 5.1.2
F004 2
F005 RL
F006 Not conducted by GLP. Few animals per group, but at a reputable
*   laboratory [Kettering Laboratory, University of Cincinnati].
F007 Not conducted by GLP. Few animals per group, but at a reputable
*   laboratory [Kettering Laboratory, University of Cincinnati].
F020 241272
EOR
F002 455
F010 5.1.2
F004 2
F005 RM
F006 Test type: Acute inhalation toxicity
**   Year: Prior to 1939
**   No. animlas/sex/group: One to two animals per dose
**   Route of administration: Inhalation
**   Dose level: 0.3%; 1%; 3%; 6% in air
**   Dose volume: N/A
**   Control: No
F007 Test type: Acute inhalation toxicity
**   Year: Prior to 1939
**   No. animlas/sex/group: One to two animals per dose
**   Route of administration: Inhalation
**   Dose level: 0.3%; 1%; 3%; 6% in air
**   Dose volume: N/A
**   Control: No
F020 241278
EOR
F002 455
F010 5.1.2
F004 2
F005 RS

F006 0.3 % (~3000 ppm)- 2 h: No visible indication of anesthetic action
**   1 and 3.0 % (~30000 ppm)- 1 h: Not lethal; signs of anesthesia
**   6.0% (~60000 ppm) : Death as the result of respiratory failure within 1 hr
F007 0.3 % (~3000 ppm)- 2 h: No visible indication of anesthetic action
**   1 and 3.0 % (~30000 ppm)- 1 h: Not lethal; signs of anesthesia
**   6.0% (~60000 ppm) : Death as the result of respiratory failure within 1 hr
F020 241264
EOR
F002 455
F010 5.1.2
F004 2
F005 TC
F006 1 or 2 hrs or until death [6%]
F007 1 or 2 hrs or until death [6%]
F020 241259
EOR
F002 455
F010 5.1.2
F004 2
F005 TS
F006 Diisopropyl ether (CAS No. 108-20-3)
**   Chemical name: Isopropyl ether; isopropoxy propane, 2-; oxybis
*   [propane], 2,2 '-
**   Test material is stated to be commercial grade with 3% of isopropyl
*   alcohol, but with no peroxide or added inhibitor.
F007 Diisopropyl ether (CAS No. 108-20-3)
**   Chemical name: Isopropyl ether; isopropoxy propane, 2-; oxybis
*   [propane], 2,2 '-
**   Test material is stated to be commercial grade with 3% of isopropyl
*   alcohol, but with no peroxide or added inhibitor.
F020 241258
EOR
F002 455
F010 5.1.2
F004 3
F005 CL
F006 The lowest lethal dose for 1 hr exposure was greater than 30,000 ppm in
*   three species.
F007 The lowest lethal dose for 1 hr exposure was greater than 30,000 ppm in
*   three species.
F020 241268
EOR
F002 455
F010 5.1.2
F004 3
F005 RE
F006 Machle W, Scott EW and Treon J (1939). The physiological response to
*   isopropyl ether and to a mixture of isopropyl ether and gasoline. J. Ind.
*   Hyg. Toxicol. 21:72-96.
F007 Machle W, Scott EW and Treon J (1939). The physiological response to
*   isopropyl ether and to a mixture of isopropyl ether and gasoline. J. Ind.
*   Hyg. Toxicol. 21:72-96.
F020 241274
EOR
F002 455
F010 5.1.2
F004 3

```
F005 RL
F006 Not conducted by GLP. Few animals per group, but at a reputable
*    laboratory [Kettering Laboratory, University of Cincinnati].
F007 Not conducted by GLP. Few animals per group, but at a reputable
*    laboratory [Kettering Laboratory, University of Cincinnati].
F020 241271
EOR
F002 455
F010 5.1.2
F004 3
F005 RM
F006 Test type:  Acute inhalation toxicity
**   Year:  Prior to 1939
**   No. animlas/sex/group:  One to two animals per dose
**   Route of administration:  Inhalation
**   Dose level:  0.3%; 1%; 3%; 6% in air
**   Dose volume:  N/A
**   Control:  No
F007 Test type:  Acute inhalation toxicity
**   Year:  Prior to 1939
**   No. animlas/sex/group:  One to two animals per dose
**   Route of administration:  Inhalation
**   Dose level:  0.3%; 1%; 3%; 6% in air
**   Dose volume:  N/A
**   Control:  No
F020 241277
EOR
F002 455
F010 5.1.2
F004 3
F005 RS
F006 0.3 % (~3000 ppm)- 2 h:  No visible indication of anesthetic action
**   1 and 3.0 % (~30000 ppm)- 1 h: Not lethal; signs of anesthesia
**   6.0% (~60000 ppm) : Death as the result of respiratory failure within 1 hr
F007 0.3 % (~3000 ppm)- 2 h:  No visible indication of anesthetic action
**   1 and 3.0 % (~30000 ppm)- 1 h: Not lethal; signs of anesthesia
**   6.0% (~60000 ppm) : Death as the result of respiratory failure within 1 hr
F020 241265
EOR
F002 455
F010 5.1.2
F004 3
F005 TC
F006 1 or 2 hrs or until death [6%]
F007 1 or 2 hrs or until death [6%]
F020 241261
EOR
F002 455
F010 5.1.2
F004 3
F005 TS
F006 Diisopropyl ether (CAS No. 108-20-3)
**   Chemical name:  Isopropyl ether; isopropoxy propane, 2-; oxybis
*    [propane], 2,2 '-
**   Test material is stated to be commercial grade with 3% of isopropyl
*    alcohol, but with no peroxide or added inhibitor.
F007 Diisopropyl ether (CAS No. 108-20-3)
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**   Chemical name:  Isopropyl ether; isopropoxy propane, 2-; oxybis
*    [propane], 2,2 '-
**   Test material is stated to be commercial grade with 3% of isopropyl
*    alcohol, but with no peroxide or added inhibitor.
F020 241260
EOR
F002 455
F010 5.1.2
F004 4
F005 CL
F006 The lowest lethal dose for 1 hr exposure was greater than 30,000 ppm in
*    three species.
F007 The lowest lethal dose for 1 hr exposure was greater than 30,000 ppm in
*    three species.
F020 241269
EOR
F002 455
F010 5.1.2
F004 4
F005 RE
F006 Machle W, Scott EW and Treon J (1939). The physiological response to
*    isopropyl ether and to a mixture of isopropyl ether and gasoline. J. Ind.
*    Hyg. Toxicol. 21:72-96.
F007 Machle W, Scott EW and Treon J (1939). The physiological response to
*    isopropyl ether and to a mixture of isopropyl ether and gasoline. J. Ind.
*    Hyg. Toxicol. 21:72-96.
F020 241275
EOR
F002 455
F010 5.1.2
F004 4
F005 RL
F006 Not conducted by GLP. Few animals per group, but at a reputable
*    laboratory [Kettering Laboratory, University of Cincinnati].
F007 Not conducted by GLP. Few animals per group, but at a reputable
*    laboratory [Kettering Laboratory, University of Cincinnati].
F020 241270
EOR
F002 455
F010 5.1.2
F004 4
F005 RM
F006 Test type:  Acute inhalation toxicity
**   Year:  Prior to 1939
**   No. animlas/sex/group:  One to two animals per dose
**   Route of administration:  Inhalation
**   Dose level:  0.3%; 1%; 3%; 6% in air
**   Dose volume:  N/A
**   Control:  No
F007 Test type:  Acute inhalation toxicity
**   Year:  Prior to 1939
**   No. animlas/sex/group:  One to two animals per dose
**   Route of administration:  Inhalation
**   Dose level:  0.3%; 1%; 3%; 6% in air
**   Dose volume:  N/A
**   Control:  No
F020 241276
```

EOR
F002 455
F010 5.1.2
F004 4
F005 RS
F006 0.3 % (~3000 ppm)- 2 h: No visible indication of anesthetic action
**   1 and 3.0 % (~30000 ppm)- 1 h: Not lethal; signs of anesthesia
**   6.0% (~60000 ppm) : Death as the result of respiratory failure within 1 hr
F007 0.3 % (~3000 ppm)- 2 h: No visible indication of anesthetic action
**   1 and 3.0 % (~30000 ppm)- 1 h: Not lethal; signs of anesthesia
**   6.0% (~60000 ppm) : Death as the result of respiratory failure within 1 hr
F020 241266
EOR
F002 455
F010 5.1.2
F004 4
F005 TC
F006 1 or 2 hrs or until death [6%]
F007 1 or 2 hrs or until death [6%]
F020 241263
EOR
F002 455
F010 5.1.2
F004 4
F005 TS
F006 Diisopropyl ether (CAS No. 108-20-3)
**   Chemical name: Isopropyl ether; isopropoxy propane, 2-; oxybis
*   [propane], 2,2 '-
**   Test material is stated to be commercial grade with 3% of isopropyl
*   alcohol, but with no peroxide or added inhibitor.
F007 Diisopropyl ether (CAS No. 108-20-3)
**   Chemical name: Isopropyl ether; isopropoxy propane, 2-; oxybis
*   [propane], 2,2 '-
**   Test material is stated to be commercial grade with 3% of isopropyl
*   alcohol, but with no peroxide or added inhibitor.
F020 241262
EOR
F002 455
F010 5.1.3
F004 2
F005 CL
F006 The test article, when administered dermally to New Zealand white rabbits
*   had an acute dermal LD50 of greater than 2.0 g/kg.
F007 The test article, when administered dermally to New Zealand white rabbits
*   had an acute dermal LD50 of greater than 2.0 g/kg.
F020 241282
EOR
F002 455
F010 5.1.3
F004 2
F005 RE
F006 Machle W, Scott EW and Treon J (1939). The physiological response to
*   isopropyl ether and to a mixture of isopropyl ether and gasoline. J. Ind.
*   Hyg. Toxicol. 21:72-96.
F007 Machle W, Scott EW and Treon J (1939). The physiological response to
*   isopropyl ether and to a mixture of isopropyl ether and gasoline. J. Ind.
*   Hyg. Toxicol. 21:72-96.

F020 241284
EOR
F002 455
F010 5.1.3
F004 2
F005 RL
F006 Not GLP but conducted at a reputable laboratory [Kettering Laboratory,
*   University of Cincinnati].
F007 Not GLP but conducted at a reputable laboratory [Kettering Laboratory,
*   University of Cincinnati].
F020 241283
EOR
F002 455
F010 5.1.3
F004 2
F005 RM
F006 Test type: Acute dermal toxicity
**   Year: Prior to 1939
**   No. of animals/sex/group: Unspecified
**   Route of administration: Dermal
**   Dose level: variable
**   Control: No
F007 Test type: Acute dermal toxicity
**   Year: Prior to 1939
**   No. of animals/sex/group: Unspecified
**   Route of administration: Dermal
**   Dose level: variable
**   Control: No
F020 241285
EOR
F002 455
F010 5.1.3
F004 2
F005 RS
F006 No deaths or systemic effects were reported. In rabbits dermal unoccluded
*   LD50 > 2.0 g/kg. The actual dose applied was much higher, but continued
*   to evaporate from the skin during application.
F007 No deaths or systemic effects were reported. In rabbits dermal unoccluded
*   LD50 > 2.0 g/kg. The actual dose applied was much higher, but continued
*   to evaporate from the skin during application.
F020 241281
EOR
F002 455
F010 5.1.3
F004 2
F005 TC
F006 The material was continuously dripped onto the shaved skin to keep it wet
*   for one hour, while continuously evaporating. 150 ml of material was used.
F007 The material was continuously dripped onto the shaved skin to keep it wet
*   for one hour, while continuously evaporating. 150 ml of material was used.
F020 241280
EOR
F002 455
F010 5.1.3
F004 2
F005 TS
F006 Diisopropyl ether (CAS No. 108-20-3)

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**   Chemical Name:  Isopropyl ether; isopropoxy propane, 2-; oxybis
*    [propane], 2,2 '-
**   Test material is stated to be commercial grade with 3% of isopropyl
*    alcohol, but with no peroxide or added inhibitor.
F007 Diisopropyl ether (CAS No. 108-20-3)
**   Chemical Name:  Isopropyl ether; isopropoxy propane, 2-; oxybis
*    [propane], 2,2 '-
**   Test material is stated to be commercial grade with 3% of isopropyl
*    alcohol, but with no peroxide or added inhibitor.
F020 241279
EOR
F002 455
F010 5.11
F004 2
F005 CL
F006 DIPE does not appear to be a sensory irritant at concentrations up to 500
*    ppm, but it does have an unpleasant odor at this concentration.
F007 DIPE does not appear to be a sensory irritant at concentrations up to 500
*    ppm, but it does have an unpleasant odor at this concentration.
F020 241327
EOR
F002 455
F010 5.11
F004 2
F005 ME
F006 Non-guideline.
F007 Non-guideline.
F020 241324
EOR
F002 455
F010 5.11
F004 2
F005 RE
F006 Silverman LH, Schulte F and First MW (1946). Further studies on sensory
*    response to certain industrial solvent vapors. J. Ind. Hyg. Toxicol.
*    28(6):262-266.
F007 Silverman LH, Schulte F and First MW (1946). Further studies on sensory
*    response to certain industrial solvent vapors. J. Ind. Hyg. Toxicol.
*    28(6):262-266.
F020 241329
EOR
F002 455
F010 5.11
F004 2
F005 RL
F006 Not GLP but conducted at a reputable laboratory [Harvard School of Public
*    Health, Boston].
F007 Not GLP but conducted at a reputable laboratory [Harvard School of Public
*    Health, Boston].
F020 241328
EOR
F002 455
F010 5.11
F004 2
F005 RM
F006 Species/strain:  Humans
**   Sex:  Male and female
```

```
**   Number/sex/group:  Average of 12
**   Route of administration:  Inhalation
**   Vehicle:  None
**   Control:  No
**   Year:  Prior to 1946
**   GLP:  No
F007 Species/strain:  Humans
**   Sex:  Male and female
**   Number/sex/group:  Average of 12
**   Route of administration:  Inhalation
**   Vehicle:  None
**   Control:  No
**   Year:  Prior to 1946
**   GLP:  No
F020 241330
EOR
F002 455
F010 5.11
F004 2
F005 RS
F006 300 ppm: 35% of the subjects objected to this solvent because of the
*    unpleasant odor rather than irritation.
**   500 ppm:  there was a sensory response that was acceptable to the
*    majority of subjects.
F007 300 ppm: 35% of the subjects objected to this solvent because of the
*    unpleasant odor rather than irritation.
**   500 ppm:  there was a sensory response that was acceptable to the
*    majority of subjects.
F020 241326
EOR
F002 455
F010 5.11
F004 2
F005 TC
F006 Subjects were exposed for 15 minutes and olfactory fatigue and irritation
*    of mucous membranes were reported. "Motion pictures were shown to occupy
*    the subject's attention and divert their thoughts from the atmospheric
*    contamination to which
F007 Subjects were exposed for 15 minutes and olfactory fatigue and irritation
*    of mucous membranes were reported. "Motion pictures were shown to occupy
*    the subject's attention and divert their thoughts from the atmospheric
*    contamination to which they were exposed."
F020 241325
EOR
F002 455
F010 5.11
F004 2
F005 TS
F006 Diisopropyl ether (CAS No. 108-20-3)
**   Chemical Name:  Isopropyl ether; isopropoxy propane, 2-; oxybis
*    [propane], 2,2 '-
**   Test material is stated to be technical grade product.
F007 Diisopropyl ether (CAS No. 108-20-3)
**   Chemical Name:  Isopropyl ether; isopropoxy propane, 2-; oxybis
*    [propane], 2,2 '-
**   Test material is stated to be technical grade product.
F020 241323
```

EOR
F002 455
F010 5.11
F004 3
F005 CL
F006 400 ppm: 5 mins of inhalation exposure caused no eye irritation, none to
* slight nose irritation, no pulmonary discomfort, olfactory recognition
* but no central nervous system effects.
**
** 800 ppm: 5 mins of inhalation exposed caused slight eye
F007 400 ppm: 5 mins of inhalation exposure caused no eye irritation, none to
* slight nose irritation, no pulmonary discomfort, olfactory recognition
* but no central nervous system effects.
**
** 800 ppm: 5 mins of inhalation exposed caused slight eye and nose
* irritation, none to slight pulmonary discomfort, definite olfactory
* recognition but no central nervous system effects.
F020 241335
EOR
F002 455
F010 5.11
F004 3
F005 ME
F006 Non-Guideline.
F007 Non-Guideline.
F020 241332
EOR
F002 455
F010 5.11
F004 3
F005 RE
F006 Hine CH, Anderson HH and Kodama JK (1955). Sensory thresholds of certain
* Shell organic solvents, Progress Report 1, Report to Shell Development
* Company, November 15, 1955. UC Report No. 247.
F007 Hine CH, Anderson HH and Kodama JK (1955). Sensory thresholds of certain
* Shell organic solvents, Progress Report 1, Report to Shell Development
* Company, November 15, 1955. UC Report No. 247.
F020 241337
EOR
F002 455
F010 5.11
F004 3
F005 RL
F006 Not GLP but conducted at a reputable laboratory [University of California
* School of Medicine].
F007 Not GLP but conducted at a reputable laboratory [University of California
* School of Medicine].
F020 241336
EOR
F002 455
F010 5.11
F004 3
F005 RM
F006 Species/strain: Young adult humans [University of California staff and
* medical students]
** Sex: Not specified
** Number/sex/group: Not specified

```
**   Route of administration:  Inhalation
**   Vehicle:  None
**   Control:  No
**   Year:  1955
**   GLP:  No
F007 Species/strain:  Young adult humans [University of California staff and
*    medical students]
**   Sex:  Not specified
**   Number/sex/group:  Not specified
**   Route of administration:  Inhalation
**   Vehicle:  None
**   Control:  No
**   Year:  1955
**   GLP:  No
F020 241338
EOR
F002 455
F010 5.11
F004 3
F005 RS
F006 Numbers of subjects with degree of effect
**   Concentration         400 ppm           800 ppm
**   Number subjects:      7                 7
**   Eye irritation:       7 absent     3 absent, 3 slight, 1 mod.
**   Nose irritation:  5 absent, 2 slight    2 abse
F007 Numbers of subjects with degree of effect
**   Concentration         400 ppm           800 ppm
**   Number subjects:      7                 7
**   Eye irritation:       7 absent     3 absent, 3 slight, 1 mod.
**   Nose irritation:  5 absent, 2 slight    2 absent, 5 slight
**   Pulmonary discomfort: 7 absent          4 absent, 3 slight
**   Olfactory cognition : 1 slight, 6 mod.  4 mod., 3 severe
**   CNS effects :         7 absent          7 absent
F020 241334
EOR
F002 455
F010 5.11
F004 3
F005 TC
F006 Exposures were conducted in a whole-body chamber approximately 7700 l
*    equipped with a fan. Exposures were made in a static atmosphere generated
*    by vaporizing a predetermined quantity of test solvent from a hot
*    surface. Five minutes were all
F007 Exposures were conducted in a whole-body chamber approximately 7700 l
*    equipped with a fan. Exposures were made in a static atmosphere generated
*    by vaporizing a predetermined quantity of test solvent from a hot
*    surface. Five minutes were allowed for evaporation and equilibration, and
*    subjects were exposed for 5 minutes, during which time they noted the
*    degree of subjective responses at one-minute intervals.
F020 241333
EOR
F002 455
F010 5.11
F004 3
F005 TS
F006 Diisopropyl ether (CAS No. 108-20-3)
**   Chemical Name:  Isopropyl ether; isopropoxy propane, 2-; oxybis
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*    [propane], 2,2 '-
**   Test material is stated to be commercial grade with purity of 98% or
*    better, provided by Shell Chemical Corporation.
F007 Diisopropyl ether (CAS No. 108-20-3)
**   Chemical Name:  Isopropyl ether; isopropoxy propane, 2-; oxybis
*    [propane], 2,2 '-
**   Test material is stated to be commercial grade with purity of 98% or
*    better, provided by Shell Chemical Corporation.
F020 241331
EOR
F002 455
F010 5.3
F004 2
F005 CL
F006 Di-isopropanol was negative in this in vitro assay.
F007 Di-isopropanol was negative in this in vitro assay.
F020 241289
EOR
F002 455
F010 5.3
F004 2
F005 RE
F006 Wass U and Belin L (1990). An in vitro method for predicting sensitizing
*    properties of inhaled chemicals. Scand. J. Work Environ. Health.
*    116:208-214.
F007 Wass U and Belin L (1990). An in vitro method for predicting sensitizing
*    properties of inhaled chemicals. Scand. J. Work Environ. Health.
*    116:208-214.
F020 241291
EOR
F002 455
F010 5.3
F004 2
F005 RL
F006 Not conducted by GLP; research method not accepted by regulatory
*    agencies; in vitro surrogate for respiratory sensitisation.
F007 Not conducted by GLP; research method not accepted by regulatory
*    agencies; in vitro surrogate for respiratory sensitisation.
F020 241290
EOR
F002 455
F010 5.3
F004 2
F005 RM
F006 Route of administration:  N/A
**   Sex:  N/A
**   Dose level:  N/A
**   Dose volume:  N/A
**   Control group included:  Positive and negative controls included
F007 Route of administration:  N/A
**   Sex:  N/A
**   Dose level:  N/A
**   Dose volume:  N/A
**   Control group included:  Positive and negative controls included
F020 241292
EOR
F002 455
```

F010 5.3
F004 2
F005 RS
F006 Diisopropanol was negative in this in vitro assay for potential
* respiratory sensitization. The assay gave positive responses with
* several known respiratory sensitizers.
F007 Diisopropanol was negative in this in vitro assay for potential
* respiratory sensitization. The assay gave positive responses with
* several known respiratory sensitizers.
F020 241288
EOR
F002 455
F010 5.3
F004 2
F005 TC
F006 A method for monitoring chemical reactivity in aqueous solutions, at
* neutral pH and 37 degrees C, was developed. The chemical was allowed to
* react with a lysine-containing peptide, and the reaction was monitored
* with high-performance liquid
F007 A method for monitoring chemical reactivity in aqueous solutions, at
* neutral pH and 37 degrees C, was developed. The chemical was allowed to
* react with a lysine-containing peptide, and the reaction was monitored
* with high-performance liquid chromatography. Simple acids, bases, and
* solvents did not react with the peptide, whereas isocyanates, anhydrides,
* and chloramine-T, substances well known for their sensitizing and asthma
* inducing properties, did. Thus a positive test strongly suggested that
* the chemical had the potential to act as a hapten and cause sensitization
* when inhaled.
F020 241287
EOR
F002 455
F010 5.3
F004 2
F005 TS
F006 Diisopropyl ether (CAS No.108-20-3)
** Chemical Name: Isopropyl ether; isopropoxy propane, 2-; oxybis
* [propane], 2,2 '-
** Source/purity not specified.
F007 Diisopropyl ether (CAS No.108-20-3)
** Chemical Name: Isopropyl ether; isopropoxy propane, 2-; oxybis
* [propane], 2,2 '-
** Source/purity not specified.
F020 241286
EOR
F002 455
F010 5.4
F004 5
F005 CL
F006 NOAEL = 480 ppm
F007 NOAEL = 480 ppm
F020 241297
EOR
F002 455
F010 5.4
F004 5
F005 ME
F006 Statistical method:

**   Statistical analyses of numerical data included ANOVA and Tukey's
*   studentized range test for data on serum chemistry. Duncan's multiple
*   range test was used for hematology and body weights to assess
*   statistically signific
F007 Statistical method:
**   Statistical analyses of numerical data included ANOVA and Tukey's
*   studentized range test for data on serum chemistry. Duncan's multiple
*   range test was used for hematology and body weights to assess
*   statistically significant differences between control and exposed groups.
F020 241294
EOR
F002 455
F010 5.4
F004 5
F005 RE
F006 Dalbey W and Fueston M (1996). Subchronic and Developmental Toxicity
*   Studies of Vaporized Diisopropyl Ether in Rats. Journal of Toxicology and
*   Environmental Health 49:29-43.
F007 Dalbey W and Fueston M (1996). Subchronic and Developmental Toxicity
*   Studies of Vaporized Diisopropyl Ether in Rats. Journal of Toxicology and
*   Environmental Health 49:29-43.
F020 241299
EOR
F002 455
F010 5.4
F004 5
F005 RL
F006 GLP unknown. Study well documented, meets generally accepted scientific
*   principles, acceptable for assessment.
F007 GLP unknown. Study well documented, meets generally accepted scientific
*   principles, acceptable for assessment.
F020 241298
EOR
F002 455
F010 5.4
F004 5
F005 RM
F006 Male and female rats were acclimated for 2 weeks before initiation of
*   exposures that began at ~8 weeks of age. Exposed animals were
*   individually housed in 1-m3 inhalation chambers. Untreated control
*   animals were housed in a separate room in
F007 Male and female rats were acclimated for 2 weeks before initiation of
*   exposures that began at ~8 weeks of age. Exposed animals were
*   individually housed in 1-m3 inhalation chambers. Untreated control
*   animals were housed in a separate room in identical caging. Room
*   environment was set to 20-22°C and 40-60% relative humidity. Lights were
*   on a 12/12-hr light/dark cycle. Food and water were provided ad libitum
*   except during exposures.
**
**   Vapors were generated by metering DIPE on to a warmed fiberglass wick and
*   carried to the three 1m3 exposure chambers by a stream of measured and
*   filtered room air. Temperature and humidity in the chambers were measured
*   every 30 minutes and air flow through each chamber was metered to provide
*   at least 12 air changes/hour. Chamber air samples were collected with a
*   gas-tight syringe and analyzed with a gas chromatograph with a flame
*   ionization detector and a fused silica column. Samples were periodically
*   obtained for analysis by gas chromatography/ mass spectroscopy.

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**
**   The primary endpoints during the course of exposures were individual body
*    weights recorded weekly and clinical signs recorded daily except on
*    weekends.
**
**   Following the last exposure, rats were fasted overnight and weighed;
*    blood samples were obtained via the orbital sinus using light anesthesia.
*    Samples were used to determine values for WBC, RBC, Hgb, Hct, MCV, MCH,
*    MCHC, platelets, and differential counts.   Glucose, urea nitrogen, total
*    protein, albumin, globulin, A/G ratio, sorbitol dehydrogenase, aspartate
*    aminotransferase, alanine aminotransferase, alkaline phosphatase, total
*    bilirubin, creatinine, cholesterol, triglycerides, uric acid, Cl, Ca, Na,
*    K, and P.  Following the collection of blood samples, all animals were
*    euthanized with sodium pentobarbital (i.p.) and exanguinated.
*    Approximately 40 tissues were collected for histopathology and organs
*    were weighed.  Testis and associated tissues were preserved whole in 10%
*    buffered formalin except for the left cauda epididymis of 10 rats in both
*    control groups and the highest test group; epididymides were evaluated
*    for morphology and number of sperm. The left testis in these groups was
*    weighed and used for determination of number of testicular spermatids.
F020 241296
EOR
F002 455
F010 5.4
F004 5
F005 RM
F006 Type:  90-Day Subchronic
**   Species/strain:  Rat/Sprague-Dawley; Tac:N(SD)fBR
**   No./sex/dose:  14/sex/group
**   Vehicle:  None
**   Method:  USEPA 1984, 40CFR Part 798:2450
F007 Type:  90-Day Subchronic
**   Species/strain:  Rat/Sprague-Dawley; Tac:N(SD)fBR
**   No./sex/dose:  14/sex/group
**   Vehicle:  None
**   Method:  USEPA 1984, 40CFR Part 798:2450
F020 241300
EOR
F002 455
F010 5.4
F004 5
F005 RS
F006 DIPE did not adversely affect clinical signs body weight, serum
*    chemistry, hematology, or the number of sperm or spermatids. Exposure to
*    males at 7100 ppm resulted in hypertrophy of liver cells associated with
*    increased liver weight and in
F007 DIPE did not adversely affect clinical signs body weight, serum
*    chemistry, hematology, or the number of sperm or spermatids. Exposure to
*    males at 7100 ppm resulted in hypertrophy of liver cells associated with
*    increased liver weight and in increased kidney weight with an increased
*    incidence of hyaline droplets in proximal tubules of the kidney. Females
*    had increased weight of both liver and kidney, although kidney increased
*    only in relation to sham-exposed controls and no morphologic changes were
*    observed in either organ. At 3300 ppm, weights of liver and kidney were
*    increased in males; the liver weights were increased in females only
*    compared to sham-exposed controls and not untreated controls. No
*    morphologic abnormalities were observed. No changes were observed with
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*    480 ppm.
F020 241295
EOR
F002 455
F010 5.4
F004 5
F005 TS
F006 Diisopropyl Ether (CAS No. 108-20-3); purity ~92%.
F007 Diisopropyl Ether (CAS No. 108-20-3); purity ~92%.
F020 241293
EOR
F002 455
F010 5.4
F004 6
F005 CL
F006 Inhalation exposures to DIPE at concentrations as high as 7060 ppm for 13
*    weeks resulted in few observable effects on the nervous system.
F007 Inhalation exposures to DIPE at concentrations as high as 7060 ppm for 13
*    weeks resulted in few observable effects on the nervous system.
F020 241305
EOR
F002 455
F010 5.4
F004 6
F005 ME
F006 Statistical method:
**   All statistical analyses were performed with SAS software.  Body weights,
*    rectal temperatures fore- and hindlimb grip strengths, the number of
*    rears, and motor activity were analyzed by a one-way analysis of variance
*    fol
F007 Statistical method:
**   All statistical analyses were performed with SAS software.  Body weights,
*    rectal temperatures fore- and hindlimb grip strengths, the number of
*    rears, and motor activity were analyzed by a one-way analysis of variance
*    followed by Duncan's multiple range test. The remaining data from the FOB
*    were analyzed by Fisher's exact test using an extended contingency table
*    containing all four groups of at given sex at a specified time. If a
*    significant difference occurred for a given parameter, Fisher's exact
*    test was used to directly compare each group individually against the
*    control. Brain weights, lengths and widths, were analyzed by Student's
*    t-test.
F020 241302
EOR
F002 455
F010 5.4
F004 6
F005 RE
F006 Rodriguez SC and Dalbey W (1997). Subchronic neurotoxicity of vaporized
*    Diisopropyl Ether in rats. International Journal of Toxicology 16:599-610.
F007 Rodriguez SC and Dalbey W (1997). Subchronic neurotoxicity of vaporized
*    Diisopropyl Ether in rats. International Journal of Toxicology 16:599-610.
F020 241307
EOR
F002 455
F010 5.4
F004 6
F005 RL
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F006 GLP unknown. Study well documented, meets generally accepted scientific
*   principles, acceptable for assessment.
F007 GLP unknown. Study well documented, meets generally accepted scientific
*   principles, acceptable for assessment.
F020 241306
EOR
F002 455
F010 5.4
F004 6
F005 RM
F006 Male and female rats were acclimated for 2 weeks before initiation of
*   exposures that began at ~8 weeks of age. Sham-exposed and exposed animals
*   were individually housed in 1-m3 inhalation chambers except during
*   behavioral testing, when they
F007 Male and female rats were acclimated for 2 weeks before initiation of
*   exposures that began at ~8 weeks of age. Sham-exposed and exposed animals
*   were individually housed in 1-m3 inhalation chambers except during
*   behavioral testing, when they were placed in another room overnight and
*   evaluated the following day. Room environment was set to 20-22ºC and
*   40-60% relative humidity. Lights were on a 12/12-hr light/dark cycle.
*   Food and water were provided ad libitum except during exposures.
*   Exposure vapors were generated by metering DIPE on to a warmed fiberglass
*   wick and carried to the three 1-m3 exposure chambers by a stream of
*   measured and filtered room air. Temperature and humidity in the chambers
*   were measured every 30 minutes and air flow through each chamber was
*   metered to provide at least 12 air changes/hour. Chamber air samples
*   were collected with a gas-tight syringe and analyzed with a gas
*   chromatograph with a flame ionization detector and a fused silica column.
*   Samples were periodically obtained for analysis by gas chromatography/
*   mass spectroscopy.
**
**   Exposures were stagger-started over a 5-day period with 16 animals,
*   2/sex/group, receiving their first exposure on each of 5 consecutive
*   days.
**
**   The rats were observed for signs of toxicity daily prior to initiation of
*   exposures, and individual body weights were recorded weekly.
**
**   During weeks of Functional Observation Battery (FOB) evaluation, four
*   rats/group would be removed from the inhalation chamber and housed
*   separately overnight and evaluated on the following day between the hours
*   of 7:30 a.m. and 11:00 a.m. The process was repeated for each consecutive
*   day until all rats were evaluated. The rats were evaluated with minimal
*   disruption to the exposure schedule and with a manageable number of rats
*   per day, 16 on any given day. The animals were evaluated in an FOB
*   followed by a determination of motor activity prior to initiation of
*   exposure; the FOB following 2, 4, 8, and 13 weeks of exposures, and for
*   motor activity following 4, 8, and 13 weeks of exposures. Following the
*   final determination of motor activity, the animals were anesthetized,
*   intravascularly perfused, and the brain, spinal cord, and peripheral
*   nerves removed for microscopic examination.
**
**   The FOB consisted of initially observing home-cage positioning, posture,
*   and reaction to removal from the cage. This was followed by evaluation
*   for exophthalmus/palpebral closure, lacrimation, salivation, pupillary
*   response, palpebral reflex, and pinna reflex. These observations were
*   scored by type and intensity. The animals were then observed for open

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*    field behavior. Piloerection, respiratory rate, tremors, convulsions,
*    posture, gait, ataxic gait, tail elevation, unperturbed activity level,
*    vocalization, number of rears, fecal balls, and urine pools were all
*    recorded during the open-field observations. Reactions to the approach of
*    a pencil, finger snap, and tail pinch were ranked and recorded. Finally,
*    fore- and hindlimb grip strength , rectal temperature , and body weight
*    were measured. Automated motor activity was assessed for 30 minutes in
*    figure-eight mazes after the completion of the FOB.
**
**   Following the last FOB and motor activity evaluation, the rats were
*    anesthetized with heparinized sodium pentobarbital (i.p.). The thoracic
*    cavity was opened and the animals were infused with phosphate-buffered
*    gluteraldehyde through the left ventricle. The perfused brain, spinal
*    cord, and sciatic nerve with its tibial, sural, and peroneal divisions
*    were removed. The brain and nerve tissues were processed for embedding in
*    paraffin or glycol methacrylate (dorsal root ganglia and peripheral
*    nerves) and sectioned for light or electron microscopic pathologic
*    evaluation.
F020 241304
EOR
F002 455
F010 5.4
F004 6
F005 RM
F006 Type:  90-Day Neurotoxicity
**   Species/strain:  Rat/Sprague-Dawley; Tac:N(SD)fBR
**   No./sex/dose:  10/sex/group
**   Vehicle:  None
**   Method:  USEPA 1984, 40CFR Part 798:6050, 6400, and 6200
F007 Type:  90-Day Neurotoxicity
**   Species/strain:  Rat/Sprague-Dawley; Tac:N(SD)fBR
**   No./sex/dose:  10/sex/group
**   Vehicle:  None
**   Method:  USEPA 1984, 40CFR Part 798:6050, 6400, and 6200
F020 241308
EOR
F002 455
F010 5.4
F004 6
F005 RS
F006 Motor activity in a figure-eight maze and unperturbed activity in the FOB
*    were decreased at week 4 in females exposed to 7060 ppm; activity in the
*    FOB was also decreased in females exposed to 450 ppm at week 4.  Other
*    changes in the FOB app
F007 Motor activity in a figure-eight maze and unperturbed activity in the FOB
*    were decreased at week 4 in females exposed to 7060 ppm; activity in the
*    FOB was also decreased in females exposed to 450 ppm at week 4.  Other
*    changes in the FOB appeared to be minor, and no changes were observed
*    during microscopic examination of tissues from the nervous system.
F020 241303
EOR
F002 455
F010 5.4
F004 6
F005 TS
F006 Diisopropyl Ether (CAS No. 108-20-3); purity ~92%.
F007 Diisopropyl Ether (CAS No. 108-20-3); purity ~92%.
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F020 241301
EOR
F002 455
F010 5.5
F004 4
F005 CL
F006 Under the conditions of this study, the test material was not mutagenic.
F007 Under the conditions of this study, the test material was not mutagenic.
F020 241311
EOR
F002 455
F010 5.5
F004 4
F005 RE
F006 Brooks TM, Meyer AL and Hutson DH (1988). The genetic toxicology of some
* hydrocarbon and oxygenated solvents. Mutagenesis 3(3):227-232.
F007 Brooks TM, Meyer AL and Hutson DH (1988). The genetic toxicology of some
* hydrocarbon and oxygenated solvents. Mutagenesis 3(3):227-232.
F020 241313
EOR
F002 455
F010 5.5
F004 4
F005 RL
F006 Restriction due to the lack of any information regarding the selection of
* dose levels used during the study. In addition no information is
* presented regarding cytotoxicity or the presence of test material
* precipitate in the cultures. Altho
F007 Restriction due to the lack of any information regarding the selection of
* dose levels used during the study. In addition no information is
* presented regarding cytotoxicity or the presence of test material
* precipitate in the cultures. Although study was not stated to be
* conducted under GLP, it was conducted at a reputable laboratory [Shell
* Research Limited, Sittingbourne Research Center].
F020 241312
EOR
F002 455
F010 5.5
F004 4
F005 RM
F006 Strains tested: Salmonella typhimurium tester strains TA98, TA100,
* TA1535, TA1537, TA1538
**
** Exposure method: Preincubation assay for volatile compounds [Brooks and
* Dean 1981]
**
** Test Substance Doses/concentration levels: Up to 8000 ug/ml i
F007 Strains tested: Salmonella typhimurium tester strains TA98, TA100,
* TA1535, TA1537, TA1538
**
** Exposure method: Preincubation assay for volatile compounds [Brooks and
* Dean 1981]
**
** Test Substance Doses/concentration levels: Up to 8000 ug/ml in the
* pre-incubation mix
**
** Metabolic activation: With and without (S9 fraction mix of livers of

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*    Aroclor 1254 pretreated rats)
**
**   Vehicle:  Tween 80/ethanol
**
**   Tester strain, activation status, Positive Controls and concentration
*    level:  Not stated
**
**   Statistical analysis:  Mean revertant colony count and standard deviation
*    were determined for each dose point.
**
**   Dose Rangefinding Study:  Cytotoxicity study
**
**   S9 Optimization Study:  No
F020 241314
EOR
F002 455
F010 5.5
F004 4
F005 RS
F006 DIPE did not induce reverse gene mutation in any strain. The test
*    substance was not genotoxic in this assay with or without metabolic
*    activation.
F007 DIPE did not induce reverse gene mutation in any strain. The test
*    substance was not genotoxic in this assay with or without metabolic
*    activation.
F020 241310
EOR
F002 455
F010 5.5
F004 4
F005 TS
F006 Diisopropyl ether (CAS No. 108-20-3)
**   Chemical Name:  Isopropyl ether; isopropoxy propane, 2-; oxybis
*    [propane], 2,2 '-
**   Source/purity not specified.
F007 Diisopropyl ether (CAS No. 108-20-3)
**   Chemical Name:  Isopropyl ether; isopropoxy propane, 2-; oxybis
*    [propane], 2,2 '-
**   Source/purity not specified.
F020 241309
EOR
F002 455
F010 5.5
F004 5
F005 CL
F006 Under the conditions of this study, the test material was not mutagenic.
F007 Under the conditions of this study, the test material was not mutagenic.
F020 242883
EOR
F002 455
F010 5.5
F004 5
F005 RE
F006 Brooks T.M., Meyer A.L. and Hutson D.H. (1988).  The genetic toxicology
*    of some hydrocarbon and oxygenated solvents. Mutagenesis, 3(3):227-232.
F007 Brooks T.M., Meyer A.L. and Hutson D.H. (1988).  The genetic toxicology
*    of some hydrocarbon and oxygenated solvents. Mutagenesis, 3(3):227-232.
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F020 242885
EOR
F002 455
F010 5.5
F004 5
F005 RL
F006 Restriction due to the lack of any information regarding the selection of
*   dose levels used during the study. In addition no information is
*   presented regarding cytotoxicity or the presence of test material
*   precipitate in the cultures. Altho
F007 Restriction due to the lack of any information regarding the selection of
*   dose levels used during the study. In addition no information is
*   presented regarding cytotoxicity or the presence of test material
*   precipitate in the cultures. Although study was not stated to be
*   conducted under GLP, it was conducted at a reputable laboratory [Shell
*   Research Limited, Sittingbourne Research Center].
F020 242884
EOR
F002 455
F010 5.5
F004 5
F005 RM
F006 Test type: Chromosome damage
**
**   Exposure method: For volatile compounds
**
**   Metabolic activation: Metabolic activation S9 was not added because
*   liver cells are metabolically competent
**
**   Vehicle: Tween 80/ethanol
**
**   Tester strain, activation sta
F007 Test type: Chromosome damage
**
**   Exposure method: For volatile compounds
**
**   Metabolic activation: Metabolic activation S9 was not added because
*   liver cells are metabolically competent
**
**   Vehicle: Tween 80/ethanol
**
**   Tester strain, activation status, Positive Controls and concentration
*   level: Cultured CHO cells were grown in 80 cm2 flasks for 24 hr before
*   compound treatment. Treatment periods were 5 hr in the presence of S9 mix
*   and 24 hr in the absence of S9. Colcemid was added to all cultures 22 hr
*   after the initial treatment. After a further 2 hr, the cells were
*   trypsinized, resuspended in hypotonic solution and then fixed, before
*   spotting onto slides. Cell preparations were then stained with Giemsa.
*   The slides were randomly coded and 100 cells from each culture were
*   analyzed microscopically. Mitotic index estimations were also made. The
*   positive controls were ethylmethanesulfonate [-S9] and cyclophosphamide
*   [+S9].
**
**   Vehicle control: Yes
**
**   Dose rangefinding study: Cytotoxicity study
**

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**   S9 Optimization study:  No
F020 242886
EOR
F002 455
F010 5.5
F004 5
F005 RS
F006 DIPE did not induce chromosomal damage in CHO cells. The test substance
*    was not genotoxic in this assay.
F007 DIPE did not induce chromosomal damage in CHO cells. The test substance
*    was not genotoxic in this assay.
F020 242882
EOR
F002 455
F010 5.5
F004 5
F005 TS
F006 Di-isopropyl ether (CAS No. 108-20-3)
**   Chemical Name:  Isopropyl ether; isopropoxy propane, 2-; oxybis
*    [propane], 2,2 '-
**   Source/purity of test material: 98.5%
F007 Di-isopropyl ether (CAS No. 108-20-3)
**   Chemical Name:  Isopropyl ether; isopropoxy propane, 2-; oxybis
*    [propane], 2,2 '-
**   Source/purity of test material: 98.5%
F020 242881
EOR
F002 455
F010 5.5
F004 6
F005 CL
F006 Under the conditions of this study, the test material was not mutagenic.
F007 Under the conditions of this study, the test material was not mutagenic.
F020 242889
EOR
F002 455
F010 5.5
F004 6
F005 RE
F006 Brooks T.M., Meyer A.L. and Hutson D.H. (1988).  The genetic toxicology
*    of some hydrocarbon and oxygenated solvents. Mutagenesis, 3(3):227-232.
F007 Brooks T.M., Meyer A.L. and Hutson D.H. (1988).  The genetic toxicology
*    of some hydrocarbon and oxygenated solvents. Mutagenesis, 3(3):227-232.
F020 242891
EOR
F002 455
F010 5.5
F004 6
F005 RL
F006 Restriction due to the lack of any information regarding the selection of
*    dose levels used during the study.  In addition no information is
*    presented regarding cytotoxicity or the presence of test material
*    precipitate in the cultures. Altho
F007 Restriction due to the lack of any information regarding the selection of
*    dose levels used during the study.  In addition no information is
*    presented regarding cytotoxicity or the presence of test material
*    precipitate in the cultures. Although study was not stated to be
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*    conducted under GLP, it was conducted at a reputable laboratory [Shell
*    Research Limited, Sittingbourne Research Center].
F020 242890
EOR
F002 455
F010 5.5
F004 6
F005 RM
F006 Test type:  Chromosome damage
**
**   Strains tested:  RL4
**
**   Metabolic activation:  Metabolic activation S9 was not added because
*    liver cells are metabolically competent.
**
**   Vehicle:  Tween 80/ethanol
**
**   Tester strain, activation status, Positive Contr
F007 Test type:  Chromosome damage
**
**   Strains tested:  RL4
**
**   Metabolic activation:  Metabolic activation S9 was not added because
*    liver cells are metabolically competent.
**
**   Vehicle:  Tween 80/ethanol
**
**   Tester strain, activation status, Positive Controls and concentration
*    level:  Cultured rat liver cells were grown and treated on glass
*    microscope slides contained in 100 ml glass Leighton tubes. After 22 hr
*    exposure to test compound or solvent, colcemid was added to each culture.
*    After a further 2 hr, the slides were removed, subjected to hypotonic
*    treatment followed by fixation and stained with Giemsa. The preparations
*    were randomly coded and 100 cells from each culture were analyzed
*    microscopically. The positive control was 7,12-dimethylbenzanthracenene.
**
**   Vehicle control:  Yes
**
**   Dose rangefinding study:  Cytotoxicity study
**
**   S9 Optimization study:  None needed
F020 242892
EOR
F002 455
F010 5.5
F004 6
F005 RS
F006 DIPE did not induce chromosomal damage in rat liver cells. The test
*    substance was not genotoxic in this assay.
F007 DIPE did not induce chromosomal damage in rat liver cells. The test
*    substance was not genotoxic in this assay.
F020 242888
EOR
F002 455
F010 5.5
F004 6
F005 TS
```

F006 Di-isopropyl ether (CAS No. 108-20-3)
** Chemical name: Isopropyl ether; isopropoxy propane, 2-; oxybis
* [propane], 2,2 '-
** Source/purity of test material: 98.5%
F007 Di-isopropyl ether (CAS No. 108-20-3)
** Chemical name: Isopropyl ether; isopropoxy propane, 2-; oxybis
* [propane], 2,2 '-
** Source/purity of test material: 98.5%
F020 242887
EOR
F002 455
F010 5.5
F004 7
F005 CL
F006 Under the conditions of this study, the test material was not genotoxic.
F007 Under the conditions of this study, the test material was not genotoxic.
F020 242895
EOR
F002 455
F010 5.5
F004 7
F005 RE
F006 Brooks T.M., Meyer A.L. and Hutson D.H. (1988). The genetic toxicology
* of some hydrocarbon and oxygenated solvents. Mutagenesis, 3(3):227-232.
F007 Brooks T.M., Meyer A.L. and Hutson D.H. (1988). The genetic toxicology
* of some hydrocarbon and oxygenated solvents. Mutagenesis, 3(3):227-232.
F020 242897
EOR
F002 455
F010 5.5
F004 7
F005 RL
F006 Restriction due to the lack of any information regarding the selection of
* dose levels used during the study. In addition no information is
* presented regarding cytotoxicity or the presence of test material
* precipitate in the cultures. Altho
F007 Restriction due to the lack of any information regarding the selection of
* dose levels used during the study. In addition no information is
* presented regarding cytotoxicity or the presence of test material
* precipitate in the cultures. Although study was not stated to be
* conducted under GLP, it was conducted at a reputable laboratory [Shell
* Research Limited, Sittingbourne Research Center].
F020 242896
EOR
F002 455
F010 5.5
F004 7
F005 RM
F006 Test type: Yeast mitotic gene conversion
**
** Strains tested: JD1
**
** Exposure method: [Brooks and Dean 1981]
**
** Metabolic activation: With and without (S9 fraction mix of livers of
* Aroclor 1254 pretreated rats)
**

```
**   Vehicle:  Tween 80/ethanol
**
**   Test
F007 Test type:  Yeast mitotic gene conversion
**
**   Strains tested:  JD1
**
**   Exposure method:  [Brooks and Dean 1981]
**
**   Metabolic activation:  With and without (S9 fraction mix of livers of
*    Aroclor 1254 pretreated rats)
**
**   Vehicle:  Tween 80/ethanol
**
**   Tester strain, activation status, Positive Controls and concentration
*    level:  Yeast cells were grown in log-phase, washed and resuspended in
*    2/5 strength YEPD broth at a concentration of 1 X 107 cells/ml. The
*    suspension was divided into 1.9 ml amounts in 30 ml universal containers
*    and 0.1 ml of test compound solution was added. For experiments with
*    metabolic activation [+S9], 0.1 ml of DIPE was added to0 1.6 ml of yeast
*    cell suspension, together with 0.3 ml of S9 mix. Initially a range of
*    concentrations of DIPE was tested up to 5 mg/ml if solubility allowed. A
*    second experiment was performed based on these results and taking into
*    account cell viability. The cultures were incubated with shaking at 30 C
*    for 18 hr. Aliquots were plated onto the appropriate culture media for
*    selection of mitotic gene convertants and cells surviving the treatment.
*    Mitotic gene conversion may be scored by supplementing the minimal medium
*    with histidine to score tryptophan prototrophs, and  with tryptophan to
*    score histidine prototrophs. Control plates were set up with solvent
*    alone and with the positive control compounds 4-nitroquinoline oxide and
*    cyclophosphamide.
**
**   Vehicle control:  Yes
**
**   Dose rangefinding study:  Cytotoxicity study
**
**   S9 Optimization study:  No
F020 242898
EOR
F002 455
F010 5.5
F004 7
F005 RS
F006 DIPE did not induce mitotic gene conversion I yeast. The test substance
*    was not genotoxic in this assay with or without metabolic activation.
F007 DIPE did not induce mitotic gene conversion I yeast. The test substance
*    was not genotoxic in this assay with or without metabolic activation.
F020 242894
EOR
F002 455
F010 5.5
F004 7
F005 TS
F006 Di-isopropyl ether (CAS No. 108-20-3)
**   Chemical name:  Isopropyl ether; isopropoxy propane, 2-; oxybis
*    [propane], 2,2 '-
**   Source/purity of test material: 98.5%
```

F007 Di-isopropyl ether (CAS No. 108-20-3)
** Chemical name: Isopropyl ether; isopropoxy propane, 2-; oxybis
* [propane], 2,2 '-
** Source/purity of test material: 98.5%
F020 242893
EOR
F002 455
F010 5.8.2
F004 2
F005 CL
F006 DIPE is not a teratogen.
F007 DIPE is not a teratogen.
F020 241319
EOR
F002 455
F010 5.8.2
F004 2
F005 ME
F006 Statistical method:
** Statistical analyses of numerical data included ANOVA and Tukey's
* studentized range test for data on serum chemistry. Duncan's multiple
* range test was used for hematology and body weights to assess
* statistically signific
F007 Statistical method:
** Statistical analyses of numerical data included ANOVA and Tukey's
* studentized range test for data on serum chemistry. Duncan's multiple
* range test was used for hematology and body weights to assess
* statistically significant differences between control and exposed groups.
* Data on the maternal biophase, cesarean sections, and fetuses were
* evaluated by ANOVA followed by group comparisons using Fisher's exact or
* Dunnett's test.
F020 241316
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F002 455
F010 5.8.2
F004 2
F005 RE
F006 Dalbey W and Fueston M (1996). Subchronic and Developmental Toxicity
* Studies of Vaporized Diisopropyl Ether in Rats. Journal of Toxicology and
* Environmental Health 49:29-43.
F007 Dalbey W and Fueston M (1996). Subchronic and Developmental Toxicity
* Studies of Vaporized Diisopropyl Ether in Rats. Journal of Toxicology and
* Environmental Health 49:29-43.
F020 241321
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F002 455
F010 5.8.2
F004 2
F005 RL
F006 GLP unknown. Study well documented, meets generally accepted scientific
* principles, acceptable for assessment.
F007 GLP unknown. Study well documented, meets generally accepted scientific
* principles, acceptable for assessment.
F020 241320
EOR
F002 455
F010 5.8.2

F004 2
F005 RM
F006 Nulliparous females were housed with males in a 1:1 ratio and observed
* daily for evidence of breeding activity. Females positive for sperm plug
* and for sperm in the vaginal lavage fluid were considered to be at day 0
* of gestation and were i
F007 Nulliparous females were housed with males in a 1:1 ratio and observed
* daily for evidence of breeding activity. Females positive for sperm plug
* and for sperm in the vaginal lavage fluid were considered to be at day 0
* of gestation and were individually housed. The females were then randomly
* distributed to 5 groups of 22 animals each: untreated controls,
* sham-exposed controls, and 3 groups exposed to vapors of DIDP at 430,
* 3095, or 6745 ppm for 6 hr/day on gestation days (GD) 6-15.
**
** Vapors were generated by metering DIPE on to a warmed fiberglass wick and
* carried to the three 1m3 exposure chambers by a stream of measured and
* filtered room air. Temperature and humidity in the chambers were measured
* every 30 minutes and air flow through each chamber was metered to provide
* at least 12 air changes/hour. Chamber air samples were collected with a
* gas-tight syringe and analyzed with a gas chromatograph with a flame
* ionization detector and a fused silica column. Samples were periodically
* obtained for analysis by gas chromatography/ mass spectroscopy.
**
** Sham-exposed and test animals were housed in their exposure chambers
* throughout the exposure period; untreated controls in a separate room.
* Food and water were not available during the 6 -hour exposure periods but
* were available ad libitum at all other times. All animals were observed
* daily. Body weights were recorded on days 0, 6, 13, 16, and 20. Food
* consumption was measured on GD 6, 13, 16, and 20. Females were sacrificed
* on GD 20 by diethyl ether overexposure followed by exsanguination. Serum
* samples from the descending aorta were analyzed for glucose, urea
* nitrogen, total protein, albumin, globulin, A/G ratio, sorbitol
* dehydrogenase, lactate dehydrogenase, aspartate aminotransferase, alanine
* aminotransferase, alkaline phosphatase, total bilirubin, creatinine,
* cholesterol, triglycerides, uric acid, Cl, Ca, Na, K, and P. All organs
* were examined grossly. The number of corpora lutea per ovary and the
* gravid uterine weights were recorded. Uterine contents were examined and
* the numbers of implantation sites, early and late resorptions, and live
* and dead fetuses were recorded. The gender of each fetus was recorded.
* Fetuses were weighed and examined for gross anomalies. Fetuses of each
* litter were equally distributed between two groups; half were fixed in
* Bouin's solution and examined for visceral anomalies and the remaining
* fetuses were fixed in 95% ethanol and examined for skeletal anomalies
* after differential staining for cartilage and bone.
**
** Dams exposed to 6745 ppm had a slight reduction in body weight gain and a
* significant decrease in food consumption. A concentration-related
* increase in the incidence of rudimentary 14th ribs was observed
* (statistically significant at 3095 and 6745 ppm) but the relevance of the
* finding was uncertain. There was no apparent toxicity, either maternal or
* fetal, at the lowest exposure concentration, 430 ppm.
F020 241318
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F010 5.8.2
F004 2
F005 RM

```
F006 Type:  Developmental Toxicity
**   Species/strain:  Sprague-Dawley; VAF/Plus Crl:CD(SD)BR
**   No./dose:  22/group
**   Vehicle:  None
**   Method:  USEPA 1984; 40CFR Part 798:4350
F007 Type:  Developmental Toxicity
**   Species/strain:  Sprague-Dawley; VAF/Plus Crl:CD(SD)BR
**   No./dose:  22/group
**   Vehicle:  None
**   Method:  USEPA 1984; 40CFR Part 798:4350
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F002 455
F010 5.8.2
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F005 RS
F006 Maternal NOEL:  430 ppm
**   Pup NOEL:  430 ppm
F007 Maternal NOEL:  430 ppm
**   Pup NOEL:  430 ppm
F020 241317
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F010 5.8.2
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F006 Diisopropyl Ether (CAS No. 108-20-3); purity ~92%.
F007 Diisopropyl Ether (CAS No. 108-20-3); purity ~92%.
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F002 1
F003 4.6.2
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F005 6
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F004 1
F005 1
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F002 1
F003 5.2.2
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F002 1
F003 5.4
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F007 11-02-2000
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F004 1
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F007 11-02-2000
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F002 1
F003 5.5
F004 2
F005 2
F006 14-01-2002
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F003 5.5
F004 3
F005 3
F006 14-01-2002
F007 11-02-2000

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F003 5.5
F004 5
F005 5
F006 11-01-2002
F007 11-02-2000
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F002 1
F003 5.7
F004 1
F005 1
F006 09-01-2002
F007 11-02-2000
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F001 27
F002 1
F003 5.8.1
F004 1
F005 1
F006 11-01-2002
F007 11-02-2000
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F001 27
F002 1
F003 5.8.2
F004 1
F005 1
F006 14-01-2002
F007 11-02-2000
EOB
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B051 DS_COMPONENT_TAB
F001 27
F002 0
F003 78-92-2
F012 N
F010 23-01-2002
F004 12032693
F005 09-01-2002
F006 12032693
F007 09-01-2002
F009 A35-01
EOR
F001 27
F002 1
F003 78-92-2
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F012 N
F010 11-02-2000
F011 11-02-2000
F004 101
F005 11-02-2000
F006 101
F007 11-02-2000
F009 A35-02
EOB
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B115 GI_COMPANY_TAB
F001 27
F002 7
F003 11-02-2000
F008 Shell Nederland Chemie B.V.
F009 P.O. Box 3030
F010 Hoogvliet-Rotterdam
F011 3190 GH
F013 A31-015
F014 +31-10-2317005
F016 +31-10-2317125
EOR
F001 27
F002 8
F003 11-02-2000
F008 Union Carbide Benelux
F009 Norderlaan 147
F010 Antwerpen
F011 2030
F013 A31-003
EOR
F001 27
F002 9
F003 11-02-2000
F008 Atochem
F009 4, Cours Michelet
F010 Paris la Defense
F011 92080
F013 A31-007
EOR
F001 27
F002 10
F003 11-02-2000
F008 SHELL FRANCE
F009 89 bld Franklin Roosevelt
F010 Rueil Malmaison
F011 92564
F013 A31-007
F014 33 1 47.14.71.00
F015 SHELL 615013F
F016 33 1 47.14.82.99
EOR
F001 27
F002 11
F003 11-02-2000
F008 EXXON CHEMICAL, Limited
F009 4600 Parkway

F010 Fareham, Hampshire
F011 PO15 7AP
F013 A31-023
F014 (44)489.88.4480
F016 (44)489.88.4455
EOR
F001 27
F002 12
F003 11-02-2000
F008 Deutsche Shell Chemie GmbH
F009 Koelner Strasse 6
F010 Eschborn
F011 65760
F013 A31-008
EOR
F001 27
F002 13
F003 11-02-2000
F008 RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
F009 Ueberseering 40
F010 Hamburg
F011 22297
F013 A31-008
F014 040-6375-0
F015 21151320
F016 040-6375-3496
EOB
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B101 GI_GENERAL_INFORM_TAB
F001 27
F002 8
F003 11-02-2000
F004 IUC300_COL
F010 A04-04
F011 A19-02
EOB
C
B102 GI_SYNONYM_TAB
F001 27
F002 1
F003 19-05-1994
F004 HEDSET
F007 2-Butanol
EOR
F001 27
F002 2
F003 19-05-1994
F004 HEDSET
F007 Ethyl methyl carbinol
EOR
F001 27
F002 3
F003 19-05-1994
F004 HEDSET
F007 2-Hydroxybutane
EOR
F001 27

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F002 4
F003 26-05-1994
F004 DS_COMPARE_PKG
F007 sec-butanol
EOR
F001 27
F002 5
F003 26-05-1994
F004 HEDSET
F007 2-butanol
EOR
F001 27
F002 6
F003 26-05-1994
F004 HEDSET
F007 secundary butyl alcohol
EOR
F001 27
F002 7
F003 27-04-1994
F004 HEDSET
F007 SBA; sec-Butanol; Butan-2-ol; secondary butyl alcohol
EOR
F001 27
F002 8
F003 20-05-1994
F004 HEDSET
F007 SBA; secondary butyl alcohol; ethyl methyl carbinol; 2-hydroxybutane
EOR
F001 27
F002 9
F003 16-02-1994
F004 DS_COMPARE_PKG
F007 SBA
EOR
F001 27
F002 11
F003 16-02-1994
F004 DS_COMPARE_PKG
F007 butan-2-ol
EOR
F001 27
F002 12
F003 16-02-1994
F004 DS_COMPARE_PKG
F007 secondary butyl alcohol
EOR
F001 27
F002 13
F003 30-05-1994
F004 HEDSET
F007 sec.-butyl alcohol, iso-butanol
EOB
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B105 GI_QUANTITY_TAB
F001 27
F002 8
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F003 11-02-2000
F004 IUC300_COL
F014 100000
F015 500000
EOB
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B106 GI_LABELLING_TAB
F001 27
F002 8
F003 11-02-2000
F004 IUC300_COL
F007 A24-01
F008 A09-09
F011 A03-02
F012 10-36/37-67
F013 2-7/9-13-24/25-26-46
F015 A12-03
F016 A12-03
EOB
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B107 GI_CLASSIFICATION_TAB
F001 27
F002 13
F003 11-02-2000
F004 IUC300_COL
F007 A08-01
F009 10
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F001 27
F002 14
F003 11-02-2000
F004 IUC300_COL
F007 A08-01
F008 A25-11
F009 36/37
EOR
F001 27
F002 15
F003 11-02-2000
F004 IUC300_COL
F007 A08-01
F009 67
EOB
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B108 GI_CATEGORY_TAB
F001 27
F002 37
F003 11-02-2000
F004 IUC300_COL
F007 A20-01
F008 A14-02
EOR
F001 27
F002 38
F003 11-02-2000
F004 IUC300_COL
F007 A20-01
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F008 A14-03
EOR
F001 27
F002 39
F003 11-02-2000
F004 IUC300_COL
F007 A20-01
F008 A14-05
EOR
F001 27
F002 40
F003 11-02-2000
F004 IUC300_COL
F007 A20-01
F008 A14-08
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F001 27
F002 41
F003 11-02-2000
F004 IUC300_COL
F007 A20-02
F008 A13-01
EOR
F001 27
F002 42
F003 11-02-2000
F004 IUC300_COL
F007 A20-02
F008 A13-02
EOR
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F002 43
F003 11-02-2000
F004 IUC300_COL
F007 A20-02
F008 A13-03
EOR
F001 27
F002 44
F003 11-02-2000
F004 IUC300_COL
F007 A20-02
F008 A13-04
EOR
F001 27
F002 45
F003 11-02-2000
F004 IUC300_COL
F007 A20-03
F008 A15-33
EOR
F001 27
F002 46
F003 11-02-2000
F004 IUC300_COL
F007 A20-03
F008 A15-48

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EOR
F001 27
F002 47
F003 11-02-2000
F004 IUC300_COL
F007 A20-03
F008 A15-55
EOR
F001 27
F002 48
F003 11-02-2000
F004 IUC300_COL
F007 A20-03
F008 A15-55: fuel additive in lead-free gasoline
EOB
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B109 GI_EXPO_LIMIT_TAB
F001 27
F002 2
F003 03-06-1994
F004 HEDSET
F007 A17-03
F008 450
F009 A16-03
EOR
F001 27
F002 3
F003 03-06-1994
F004 HEDSET
F007 A17-07
F008 303
F009 A16-03
EOR
F001 27
F002 4
F003 26-05-1994
F004 HEDSET
F007 A17-07
F008 303
F009 A16-03
F010 455
F011 A16-03
EOR
F001 27
F002 5
F003 27-04-1994
F004 HEDSET
F007 A17-07
F008 303
F009 A16-03
F010 455
F011 A16-03
F012 15
F013 A18-02
F014 4
EOR
F001 27
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F002 6
F003 27-04-1994
F004 HEDSET
F007 A17-04
F008 300
F009 A16-03
F010 600
F011 A16-03
F012 30
F013 A18-02
F014 4
EOR
F001 27
F002 7
F003 27-04-1994
F004 HEDSET
F007 A17-09: VME
F008 300
EOR
F001 27
F002 8
F003 26-05-1994
F004 HEDSET
F007 A17-07
F008 303
F009 A16-03
EOR
F001 27
F002 9
F003 16-02-1994
F004 DS_COMPARE_PKG
F007 A17-07
F008 303
F009 A16-03
F010 455
F011 A16-03
F012 8
F013 A18-01
EOR
F001 27
F002 10
F003 16-02-1994
F004 DS_COMPARE_PKG
F007 A17-04
F008 300
F009 A16-03
EOR
F001 27
F002 11
F003 16-02-1994
F004 HEDSET
F007 A17-03
F008 450
F009 A16-03
EOR
F001 27
F002 12
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F003 16-02-1994
F004 DS_COMPARE_PKG
F007 A17-06
F008 300
F009 A16-03
F010 450
F011 A16-03
EOR
F001 27
F002 13
F003 30-05-1994
F004 HEDSET
F007 A17-04
F008 100
F009 A16-04
EOR
F001 27
F002 16
F003 13-05-1994
F004 HEDSET
F007 A17-03
F008 450
F009 A16-03
EOB
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B110 GI_SOURCE_OF_EXPOSURE_TAB
F001 27
F002 1
F003 24-05-1994
F004 HEDSET
EOR
F001 27
F002 2
F003 03-06-1994
F004 HEDSET
EOR
F001 27
F002 3
F003 23-02-1994
F004 HEDSET
EOB
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B114 GI_OTHER_TAB
F001 27
F002 1
F003 10-06-1994
F004 HEDSET
EOR
F001 27
F002 2
F003 26-05-1994
F004 HEDSET
EOR
F001 27
F002 3
F003 26-05-1994
F004 HEDSET
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F001 27
F002 4
F003 30-05-1994
F004 HEDSET
EOB
C
B201 PC_MELTING_TAB
F001 27
F002 1
F003 17-01-2002
F004 DAWINKE
F016 2
F007 A02-06
F008 -89
F009 -108
F012 P01-03: no data
F014 A03-02
EOR
F001 27
F002 2
F003 17-01-2002
F004 DAWINKE
F016 1
F007 A02-03
F008 -114
F012 P01-03: no data
F014 A03-02
EOB
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B202 PC_BOILING_TAB
F001 27
F002 1
F003 17-01-2002
F004 DAWINKE
F017 2
F007 A02-06
F008 99
F009 102
F010 1013
F011 P02-01
F013 P03-03: ASTM D1078/86
F014 1986
F015 A03-02
EOR
F001 27
F002 2
F003 17-01-2002
F004 DAWINKE
F017 1
F007 A02-03
F008 99.5
F013 P03-03: no data
F015 A03-02
EOB
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B203 PC_DENSITY_TAB
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F001 27
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F004 DAWINKE
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F007 P05-02
F008 A02-06
F009 807
F011 P18-02
F012 15
F013 P04-03: ASTM D4052/86
F014 1986
F015 A03-02
EOR
F001 27
F002 2
F003 17-01-2002
F004 DAWINKE
F007 P05-02
F008 A02-03
F009 3.29
F011 P18-02
F012 20
F013 P04-03: no data
F015 A03-02
EOR
F001 27
F002 3
F003 17-01-2002
F004 DAWINKE
F017 1
F007 P05-02
F008 A02-03
F009 806
F011 P18-02
F012 20
F013 P04-03: no data
F015 A03-02
EOB
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B204 PC_VAPOUR_TAB
F001 27
F002 1
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F004 DAWINKE
F016 1
F007 A02-03
F008 15.98
F010 P02-01
F011 20
F012 P06-04
F014 A03-02
EOB
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B205 PC_PARTITION_TAB
F001 27
F002 2
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F003 17-01-2002
F004 DAWINKE
F015 1
F007 A02-03
F008 .61
F010 20
F011 P07-05
F013 A03-02
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B206 PC_WATER_SOL_TAB
F001 27
F002 1
F003 17-01-2002
F004 DAWINKE
F024 3
F007 A02-06
F008 P08-01
F009 201
F011 20
F020 P09-03: no data
F022 A03-02
EOR
F001 27
F002 2
F003 17-01-2002
F004 DAWINKE
F024 1
F007 A02-03
F008 P08-01
F009 125
F011 20
F020 P09-03: no data
F022 A03-02
EOR
F001 27
F002 3
F003 17-01-2002
F004 DAWINKE
F024 2
F007 A02-03
F008 P08-01
F009 181
F011 25
F020 P09-03: no data
F022 A03-02
EOB
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B207 PC_FLASH_TAB
F001 27
F002 1
F003 01-06-1994
F004 HEDSET
F007 A02-06
F008 25
F009 P10-01
F010 P11-01
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F011 1987
F012 A03-02
EOR
F001 27
F002 2
F003 17-01-2002
F004 DAWINKE
F014 1
F007 A02-03
F008 24
F009 P10-01
F010 P11-02: NFT 60 103
F012 A03-02
EOB
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B208 PC_AUTO_FLAMM_TAB
F001 27
F002 1
F003 17-01-2002
F004 DAWINKE
F016 1
F007 A02-04
F008 350
F010 1013
F011 P02-01
F012 P13-03: E695/85
F013 1985
F014 A03-02
EOR
F001 27
F002 2
F003 02-06-1994
F004 HEDSET
F007 A02-03
F008 406
F010 1013
F011 P02-01
F012 P13-03: no data
F014 A03-02
EOB
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B209 PC_FLAMM_TAB
F001 27
F002 1
F003 17-01-2002
F004 DAWINKE
F012 1
F007 P16-04
F008 P15-05: no data
F010 A03-02
EOB
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B210 PC_EXPL_TAB
F001 27
F002 1
F003 17-01-2002
F004 DAWINKE

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F012 1
F008 P21-02: no data
F010 A03-02
EOB
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B301 EN_PHOTODEGRADATION_TAB
F001 27
F002 1
F003 18-01-2002
F004 DAWINKE
F046 5
EOR
F001 27
F002 4
F003 17-01-2002
F004 DAWINKE
F046 4
F008 F01-01
F009 F02-06
F011 F03-03: sun lamp
F043 A03-02
EOR
F001 27
F002 5
F003 17-01-2002
F004 DAWINKE
F046 3
F008 F01-01
F009 F02-04
F010 1990
F034 F06-03
F035 1000000
F036 F07-02
F044 A02-03
F037 .0000000000096466
F038 A02-03
F040 50
F041 20
F042 F05-02
EOR
F001 27
F002 6
F003 17-01-2002
F004 DAWINKE
F045 A36-003
F046 1
F008 F01-01
F009 F02-05
F034 F06-03
F035 1500000
F036 F07-02
F044 A02-03
F037 .0000000000099751
F038 A02-03
F040 50
F041 12.9
F042 F05-02
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F001 27
F002 7
F003 17-01-2002
F004 DAWINKE
F046 2
F008 F01-01
F009 F02-06
F034 F06-03
F043 A03-02
EOB
C
B302 EN_STABILITY_IN_WATER_TAB
F001 27
F002 2
F003 17-01-2002
F004 DAWINKE
F041 1
F008 F08-01
F039 A03-02
EOB
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B303 EN_STABILITY_IN_SOIL_TAB
F001 27
F002 1
F003 18-01-2002
F004 DAWINKE
F055 1
EOB
C
B304 EN_MONITORING_TAB
F001 27
F002 1
F003 17-01-2002
F004 DAWINKE
F010 6
F007 F19-01
F008 F35-09
EOR
F001 27
F002 2
F003 17-01-2002
F004 DAWINKE
F010 1
F007 F19-01
F008 F35-07
EOR
F001 27
F002 3
F003 17-01-2002
F004 DAWINKE
F010 4
F007 F19-02
F008 F35-08: wastewater
EOR
F001 27
F002 4
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F003 17-01-2002
F004 DAWINKE
F010 5
F007 F19-02
F008 F35-08: landfill leachate
EOR
F001 27
F002 5
F003 17-01-2002
F004 DAWINKE
F010 2
F007 F19-01
F008 F35-01
EOR
F001 27
F002 6
F003 17-01-2002
F004 DAWINKE
F010 3
F007 F19-01
F008 F35-01
EOB
C
B305 EN_TRANSPORT_TAB
F001 27
F002 1
F003 17-01-2002
F004 DAWINKE
F012 1
F007 F20-03
F008 F22-03
F009 F21-01
EOB
C
B306 EN_DISTRIBUTION_TAB
F001 27
F002 1
F003 17-01-2002
F004 DAWINKE
F010 A36-003
F011 1
F007 F24-02
F008 F23-01
EOB
C
B308 EN_BIODEGRADATION_TAB
F001 27
F002 2
F003 14-01-2002
F004 CLGETTS
F048 7
F007 A01-01
F008 F25-01
F011 F27-0166: semi-automatic activated sludge system
F020 F30-02: 98% BOD reduction after 5 days
F046 A03-02
EOR
```

F001 27
F002 3
F003 14-01-2002
F004 CLGETTS
F048 9
F007 A01-01
F008 F25-02
F011 F27-0166: acetate-acclimated methane cultures
F017 100
F018 14
F019 F05-01
F046 A03-02
EOR
F001 27
F002 4
F003 14-01-2002
F004 CLGETTS
F048 8
F007 A01-01
F008 F25-02
F011 F27-0166: acetate enriched cultures
F046 A03-02
EOR
F001 27
F002 5
F003 17-01-2002
F004 DAWINKE
F048 5
F008 F25-01
F009 F26-25: screening test
F011 F27-0137
F015 A02-03
F017 33
F018 5
F019 F05-01
F046 A03-02
EOR
F001 27
F002 7
F003 17-01-2002
F004 DAWINKE
F048 4
F008 F25-01
F009 F26-25: screening test
F011 F27-0137
F015 A02-03
F017 81.7
F018 5
F019 F05-01
F046 A03-02
EOR
F001 27
F002 8
F003 17-01-2002
F004 DAWINKE
F048 6
F008 F25-01

```
F009 F26-25: screening test
F011 F27-0137
F015 A02-03
F017 9.3
F018 1
F019 F05-01
F046 A03-02
EOR
F001 27
F002 9
F003 17-01-2002
F004 DAWINKE
F048 3
F008 F25-01
F009 F26-25: screening test
F011 F27-0137
F015 A02-03
F017 98.5
F018 5
F019 F05-01
F046 A03-02
EOR
F001 27
F002 10
F003 18-01-2002
F004 DAWINKE
F047 A36-003
F048 1
F008 F25-01
F009 F26-25:  APHA (American Public Health Association) Standard Methods, No.
*    219
F011 F27-0166:  Wastewater treatment plant
F015 A02-03
F017 83
F018 5
F019 F05-01
F046 A03-02
F052 5
F053 F05-01
EOR
F001 27
F002 11
F003 18-01-2002
F004 DAWINKE
F047 A36-003
F048 2
F009 F26-25:  Winkler Method
F011 F27-0166:  Wastewater treatment plant
F046 A03-02
F052 50
F053 F05-01
EOB
C
B309 EN_BOD_COD_TAB
F001 27
F002 1
F003 17-01-2002
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F004 DAWINKE
F023 1
F007 F32-03: not specified
F009 A03-02
F013 A02-03
F014 1.87
F015 F33-03: not specified
F017 A03-02
F018 A02-03
F019 2.47
F020 A02-03
F021 .76
EOB
C
B310 EN_BIOACCUMULATION_TAB
F001 27
F002 1
F003 18-01-2002
F004 DAWINKE
F022 1
F009 F34-06: calculated value
F016 A02-06
F017 1.71
F020 A03-02
EOB
C
B311 EN_OTHER_TAB
F001 27
F002 1
F003 17-01-2002
F004 DAWINKE
F010 1
F009 The volatilization half-life in a model river is estimated to be 3.5 days
*    at 25 degrees C.
EOB
C
B401 EC_FISHTOX_TAB
F001 27
F002 3
F003 17-01-2002
F004 DAWINKE
F034 3
F008 E01-05
F009 E02-0075
F010 E03-05: not specified
F012 48
F013 E04-02
F014 E05-02
F021 A02-03
F022 3520
F031 A03-01
F032 A03-02
F045 E35-02
EOR
F001 27
F002 4
F003 18-01-2002
```

F004 DAWINKE
F034 4
F008 E01-05
F009 E02-0113
F010 E03-05: not specified
F012 24
F013 E04-02
F031 A03-01
F032 A03-02
EOR
F001 27
F002 5
F003 18-01-2002
F004 DAWINKE
F033 A36-003
F034 1
F007 A01-01
F008 E01-02
F009 E02-0119
F010 E03-05: no data
F011 1985
F012 96
F013 E04-02
F014 E05-02
F021 A02-03
F022 3670
F031 A03-03
F032 A03-02
F045 E35-02
EOR
F001 27
F002 6
F003 17-01-2002
F004 DAWINKE
F033 A36-003
F034 2
F008 E01-05
F009 E02-0015
F010 E03-05: APHA (American Public Health Association) Standard Methods
F012 24
F013 E04-02
F014 E05-02
F021 A02-03
F022 4300
F031 A03-03
F032 A03-02
F045 E35-02
EOR
F001 27
F002 7
F003 17-01-2002
F004 DAWINKE
F033 A36-003
F034 5
F009 E02-0161: fish
F010 E03-05: ECOSAR Computer Model
F012 96

```
F013 E04-02
F014 E05-02
F021 A02-03
F022 1113
F045 E35-01
EOB
C
B402 EC_DAPHNIATOX_TAB
F001 27
F002 1
F003 17-01-2002
F004 DAWINKE
F033 2
F008 E06-0010
F009 E07-04: not specified
F011 24
F012 E04-02
F013 E05-02
F026 LC50
F027 A02-03
F028 3750
F030 A03-01
F031 A03-02
F042 E01-05
F047 E35-02
EOR
F001 27
F002 2
F003 18-01-2002
F004 DAWINKE
F032 A36-003
F033 1
F007 A01-01
F008 E06-0010
F009 E07-04:  German Institute of Standardization, DIN 38412, Part II, Daphnia
*    Short-Time Test
F011 48
F012 E04-02
F013 E05-02
F020 A02-03
F021 4227
F030 A03-01
F031 A03-02
F042 E01-05
F045 E35-02
EOR
F001 27
F002 3
F003 17-01-2002
F004 DAWINKE
F032 A36-003
F033 3
F008 E06-0034:  Tetrahymena pyrifomis (Ciliate)
F009 E07-04:  Population Growth Impairment Test
F011 48
F012 E04-02
F013 E05-02
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F020 A02-03
F021 3196
F030 A03-02
F031 A03-02
F042 E01-05
F045 E35-02
EOR
F001 27
F002 4
F003 17-01-2002
F004 DAWINKE
F032 A36-003
F033 4
F008 E06-0034: Daphnid
F009 E07-04:  ECOSAR Computer Model
F011 48
F012 E04-02
F013 E05-02
F026 LC50
F027 A02-03
F028 1084
F047 E35-01
EOB
C
B403 EC_ALGAETOX_TAB
F001 27
F002 2
F003 18-01-2002
F004 DAWINKE
F037 4
F008 E08-0037
F009 E09-04: not specified
F012 192
F013 E04-02
F014 E05-02
F015 A02-03
F016 312
F034 A03-02
F035 A03-02
F046 E35-02
EOR
F001 27
F002 3
F003 18-01-2002
F004 DAWINKE
F037 5
F008 E08-0018
F009 E09-04: not specified
F014 E05-02
F015 A02-03
F016 8900
F034 A03-02
F035 A03-02
F046 E35-02
EOR
F001 27
F002 4
```

F003 17-01-2002
F004 DAWINKE
F036 A36-003
F037 1
F008 E08-0053
F009 E09-04: 7-Day Cell Multiplication Inhibition Test
F012 7
F013 E04-01
F014 E05-02
F030 TT
F031 A02-03
F032 95
F034 A03-01
F035 A03-02
F051 E35-02
EOR
F001 27
F002 5
F003 17-01-2002
F004 DAWINKE
F036 A36-003
F037 2
F008 E08-0063: green alga
F009 E09-04: ECOSAR Computer Model
F012 96
F013 E04-02
F014 E05-02
F027 A02-03
F028 625
F050 E35-01
EOR
F001 27
F002 6
F003 18-01-2002
F004 DAWINKE
F036 A36-003
F037 3
F009 E09-04: ECOSAR Computer Model
F011 E10-03: green alga
F012 96
F013 E04-02
F014 E05-02
F030 ChV*
F031 A02-03
F032 28
F051 E35-01
EOB
C
B404 EC_BACTOX_TAB
F001 27
F002 1
F003 18-01-2002
F004 DAWINKE
F035 1
F008 E29-01
F009 E11-0109
F010 E12-06: total biomass

F012 16
F013 E04-02
F014 E05-02
F015 A02-06
F016 500
F024 NOAEL
F025 A02-03
F026 500
F032 A03-02
F033 A03-02
F036 E35-02
EOR
F001 27
F002 2
F003 18-01-2002
F004 DAWINKE
F035 2
F009 E11-0029
F014 E05-02
F021 A02-03
F022 1630
F032 A03-02
F033 A03-02
F038 E35-02
EOR
F001 27
F002 3
F003 17-01-2002
F004 DAWINKE
F035 5
F008 E29-01
F009 E11-0140
F010 E12-06: total biomass
F012 20
F013 E04-02
F014 E05-02
F024 NOEC
F025 A02-03
F026 1416
F032 A03-02
F033 A03-02
EOR
F001 27
F002 4
F003 18-01-2002
F004 DAWINKE
F035 3
F008 E29-01
F009 E11-0037
F010 E12-06: total biomass
F012 48
F013 E04-02
F014 E05-02
F024 NOEL
F025 A02-03
F026 745
F032 A03-02

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F033 A03-02
F039 E35-02
EOR
F001 27
F002 5
F003 18-01-2002
F004 DAWINKE
F035 4
F008 E29-01
F009 E11-0054
F010 E12-06: total biomass
F012 72
F013 E04-02
F014 E05-02
F024 NOEL
F025 A02-03
F026 1282
F032 A03-02
F033 A03-02
F039 E35-02
EOB
C
B405 EC_CHRONFISHTOX_TAB
F001 27
F002 1
F003 17-01-2002
F004 DAWINKE
F030 A36-003
F031 1
F008 E02-0161: fish
F009 E13-02:  ECOSAR Computer Model
F012 30
F013 E15-01
F014 E05-02
F024 ChV*
F025 A02-03
F026 115
F035 E35-01
EOB
C
B406 EC_CHRONDAPHNIATOX_TAB
F001 27
F002 1
F003 17-01-2002
F004 DAWINKE
F030 A36-003
F031 1
F008 E06-0034: Daphnid
F009 E16-02:  ECOSAR Computer Model
F012 16
F013 E18-01
F014 E05-02
F015 A02-03
F016 30
F032 E35-01
EOB
C
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B408 EC_PLANTTOX_TAB
F001 27
F002 1
F003 17-01-2002
F004 DAWINKE
F034 5
F008 E23-06
F009 E24-02: not indicated
F011 E25-03: seed germination
F014 E05-02
F018 A02-03
F019 650
F032 A03-02
EOR
F001 27
F002 2
F003 17-01-2002
F004 DAWINKE
F034 6
F008 E23-17: Cucumis sativus
F009 E24-02: not specified
F011 E25-03: seed germination
F014 E05-02
F015 A02-01
F016 50375
F032 A03-02
EOR
F001 27
F002 3
F003 17-01-2002
F004 DAWINKE
F034 4
F008 E23-17: Lupinus albus
F012 1
F013 E15-01
F032 A03-02
EOR
F001 27
F002 4
F003 17-01-2002
F004 DAWINKE
F034 1
F008 E23-17: Solanum tuberosum L.
F032 A03-02
EOR
F001 27
F002 5
F003 17-01-2002
F004 DAWINKE
F034 3
F008 E23-17: wheat
F032 A03-02
EOR
F001 27
F002 6
F003 17-01-2002
F004 DAWINKE

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F034 2
F008 E23-17: wheat
F032 A03-02
EOB
C
B407 EC_SOILDWELLINGTOX_TAB
F001 27
F002 1
F003 17-01-2002
F004 DAWINKE
F033 A36-003
F034 1
F009 E20-0039: earthworm
F010 E21-03:  ECOSAR Computer Model
F012 E22-01
F013 14
F014 E04-01
F015 E33-03: ppm
F022 A02-03
F023 1222
F037 E35-01
EOB
C
B409 EC_OTHER_SPEC_TAB
F001 27
F002 2
F003 18-01-2002
F004 DAWINKE
F032 A36-003
F008 E26-15:  Xenopus laevis (Clawed Frog)
F009 E27-03:  not specified
F011 E28-01
F012 48
F013 E30-03
F014 E32-02:  mg/L
F021 A02-03
F022 1530
F031 A03-02
F036 E35-02
EOB
C
B017 TO_META_MAM_TAB
F001 27
F002 1
F003 01-06-2006
F004 CLGETTS
F005 A36-002
F006 1
F009 T02-24
F021 T52-003:  Aqueous Solution
F022 C34-001:  Oral Gavage / i.v.
F034 C36-001:  Experimental Model Development
F035 1981
F036 A03-02
F037 A01-03:  2-Butanol (sec-Butanol; sBA) and metabolites 2-Butanone (Methyl
*    ethyl ketone; MEK), 3-Hydroxy-2-Butanone (3H-2B), and 2,3-Butanediol
*    (2,3-BD) (CAS Nos. 78-92-2 (sBA); 78-93-3 (MEK))
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F042 (See Remark)
EOR
F001 27
F002 2
F003 01-06-2006
F004 CLGETTS
F005 A36-002
F006 2
F009 T02-10
F021 T52-003: Corn oil (25% solution)
F022 C34-003
F034 C36-001: Experimental
F035 1976
F036 A03-02
F037 A01-03: 2-Butanone (Methyl ethyl ketone; MEK) (CAS No. 78-93-3)
F042 450 mg/kg body weight
EOR
F001 27
F002 3
F003 01-06-2006
F004 CLGETTS
F005 A36-002
F006 3
F009 T02-13
F010 9
F021 T52-003: none
F022 C34-010
F034 C36-001: Experimental
F035 1988
F036 A03-02
F037 A01-03: 2-Butanone (Methyl ethyl ketone; MEK) (CAS No. 78-93-3)
F042 200 ppm (8.2mmol/m3)
EOB
C
B501 TO_ACUTE_ORAL_TAB
F001 27
F002 1
F003 21-10-1992
F004 HEDSET
F007 A01-01
F008 T01-03
F009 T02-24
F010 T03-03
F012 A02-03
F013 6500
F015 T04-01
F016 A03-02
EOR
F001 27
F002 2
F003 21-10-1992
F004 HEDSET
F007 A01-01
F008 T01-03
F009 T02-23
F010 T03-03: not specified
F011 1972

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F012 A02-03
F013 4900
F015 T04-01
F016 A03-02
EOR
F001 27
F002 3
F003 10-01-2002
F004 CLGETTS
F017 A36-002
F007 A01-01
F008 T01-03
F009 T02-24
F010 T03-03:  Experimental (Non-regulatory)
F011 1986
F012 A02-03
F013 2054
F014 2328
F015 T04-01
F016 A03-03
F019 T24-03
F020 10
F021 T52-003:  None
F022 T23-16
EOR
F001 27
F002 4
F003 10-01-2002
F004 CLGETTS
F017 A36-003
F007 A01-01
F008 T01-03
F009 T02-24
F010 T03-03:  Experimental (Non-regulatory)
F011 1954
F012 A02-03
F013 5730
F014 7320
F015 T04-01
F016 A03-01
F019 T24-02
F020 5
F021 T52-003:  Unknown (water, corn oil, or a 1% solution of
*    3,9-diethyl-6-tridecanol sulfate (Tergitol Penetrant 7)
F022 T23-48:  Carworth-Wistar
EOR
F001 27
F002 5
F003 10-01-2002
F004 CLGETTS
F017 A36-004
F007 A01-01
F008 T01-03
F009 T02-23
F010 T03-03:  Experimental (Non-regulatory)
F011 1925
F012 A02-03
```

F013 4890
F015 T04-01
F016 A03-01
F019 T24-03
F021 T52-002
F022 T23-48: Unknown
EOB
C
B502 TO_ACUTE_INHAL_TAB
F001 27
F002 1
F003 11-01-2002
F004 CLGETTS
F019 A36-003
F007 A01-01
F008 T05-03
F009 T02-24
F010 T06-03: Experimental (Non-regulatory)
F011 1954
F012 A02-03
F013 16000
F015 T07-02
F016 4
F017 T08-01
F018 A03-01
F021 T24-02
F022 6
F023 T52-003: None
F024 T23-48: Carworth-Wistar
EOR
F001 27
F002 2
F003 10-01-2002
F004 CLGETTS
F019 A36-003
F007 A01-01
F008 T05-03
F009 T02-24
F010 T06-03: Experimental (Non-regulatory)
F011 1951
F012 A02-03
F013 8000
F015 T07-02
F016 4
F017 T08-01
F018 A03-01
F021 T24-02
F022 6
F023 T52-003: None
F024 T23-48: Carworth-Wistar
EOR
F001 27
F002 3
F003 10-01-2002
F004 CLGETTS
F019 A36-003
F007 A01-01

F008 T05-03
F009 T02-24
F010 T06-03: Experimental (Non-regulatory)
F011 1989
F012 A02-03
F013 10000
F015 T07-02
F016 7
F017 T08-01
F018 A03-03
F021 T24-01
F022 5
F023 T52-003: None
F024 T23-42
EOR
F001 27
F002 4
F003 10-01-2002
F004 CLGETTS
F019 A36-005
F007 A01-01
F008 T05-03
F009 T02-18
F010 T06-03: Experimental (Non-regulatory)
F011 1938
F018 A03-01
F021 T24-04
F022 2
F023 T52-003: None
F024 T23-47
EOB
C
B503 TO_ACUTE_DERMAL_TAB
F001 27
F002 1
F003 10-01-2002
F004 CLGETTS
F017 A36-002
F007 A01-01
F008 T01-05: Limit
F009 T02-24
F010 T09-02: Experimental (Non-regulatory)
F011 1986
F012 A02-04
F013 2000
F015 T04-01
F016 A03-03
F019 T24-03
F020 10
F021 T52-003: None
F022 T23-16
EOB
C
B504 TO_ACUTE_OTHER_TAB
F001 27
F002 1
F003 21-10-1992

F004 HEDSET
F007 A01-01
F008 T10-07
F009 T02-18
F010 T11-02
F011 other: not specified
F012 1978
F013 A02-03
F014 800
F016 T12-01
F019 A03-02
EOB
C
B505 TO_SKIN_IRRITATION_TAB
F001 27
F002 1
F003 21-10-1992
F004 HEDSET
F007 A01-01
F008 T02-23
F009 T14-06: not specified
F010 1954
F011 T15-04
F012 T46-06
F013 A03-02
EOR
F001 27
F002 2
F003 10-01-2002
F004 CLGETTS
F014 A36-002
F007 A01-01
F008 T02-23
F009 T14-05
F010 1986
F011 T15-04
F012 T46-06
F013 A03-03
F018 T50-001
F019 4
F020 T55-001
F021 6
EOB
C
B506 TO_EYE_IRRITATION_TAB
F001 27
F002 1
F003 10-01-2002
F004 CLGETTS
F014 A36-003
F007 A01-01
F008 T02-23
F009 T16-04: Experimental (Non-regulatory)
F010 1954
F011 T17-01
F012 T46-04
F013 A03-01

F022 5
EOR
F001 27
F002 2
F003 10-01-2002
F004 CLGETTS
F014 A36-002
F007 A01-01
F008 T02-23
F009 T16-03
F010 1986
F012 T46-01
F013 A03-03
F022 6
EOB
C
B507 TO_SENSITIZATION_TAB
F001 27
F002 1
F003 11-01-2002
F004 CLGETTS
F015 A36-002
F007 A01-01
F008 T18-03
F009 T02-10
F010 T20-03: Magnusson and Kligman; 1969
F011 1986
F012 T47-01
F013 T21-02
F014 A03-03
F017 20
F030 T52-003: Corn oil
EOR
F001 27
F002 2
F003 11-01-2002
F004 CLGETTS
F015 A36-002
F007 A01-03
F008 T18-04
F009 T02-10
F010 T20-03: OECD Guide-line 406 and EC92/69/EEC, B6
F011 1992
F012 T47-01
F013 T21-02
F014 A03-03
F017 20
F030 T52-003: Paraffin oil
EOB
C
B508 TO_REPEATED_DOSE_TAB
F001 27
F002 1
F003 14-01-2002
F004 CLGETTS
F030 A36-002
F031 2

F007 A01-03
F008 T02-24
F009 T23-16
F010 T24-03
F011 T25-08
F012 T26-16: Comparable to OECD Guideline 413; 90-Day Subchronic Toxicity
F013 1981
F014 90 days
F015 6 hours/day; 5 days/week
F017 0, 1250, 2500, or 5000 ppm - Vapor
F018 T27-07
F019 A02-03
F020 2500
F022 T28-05
F024 A02-03
F025 5000
F027 T28-05
F029 A03-03
EOR
F001 27
F002 2
F003 11-01-2002
F004 CLGETTS
F030 A36-003
F031 1
F007 A01-01
F008 T02-24
F009 T23-42
F010 T24-02
F011 T25-08
F012 T26-16: Experimental -- Study of changes in cytochrome P-450 enzyme
*   system of rat liver, kidney and lung
F013 1985
F014 3-5 days
F015 6 hours/day
F017 2000 ppm (3 Days) and 500 ppm (5 Days)
F029 A03-02
EOB
C
B509 TO_GENETIC_IN_VITRO_TAB
F001 27
F002 1
F003 11-01-2002
F004 CLGETTS
F016 A36-002
F007 A01-01
F008 T30-01
F009 T31-10
F010 1985
F011 Bacterial
F012 T32-03
F013 T33-02
F014 A03-03
F015 0.01, 0.1, 0.5, 1.0, and 5.0 mg/ml
EOR
F001 27
F002 2

F003 14-01-2002
F004 CLGETTS
F016 A36-002
F007 A01-01
F008 T30-01
F009 T31-11
F010 1985
F011 Bacterial
F012 T32-03
F013 T33-02
F014 A03-03
F015 0.01, 0.1, 0.5, 1.0, and 5.0 mg/ml
EOR
F001 27
F002 3
F003 14-01-2002
F004 CLGETTS
F016 A36-002
F007 A01-01
F008 T30-19: Yeast mitotic gene conversion
F009 T31-16
F010 1988
F011 Saccharomyces cerevisiae
F012 T32-03
F013 T33-02
F014 A03-03
F015 Maximum conc. 5 mg/ml
EOR
F001 27
F002 4
F003 14-01-2002
F004 CLGETTS
F016 A36-002
F007 A01-01
F008 T30-19: chromosome abberration assay
F009 T31-12
F010 1988
F011 Chinese hamster ovary cells
F012 T32-03
F013 T33-02
F014 A03-03
F015 maximum conc. 5000 ug/ml
EOR
F001 27
F002 5
F003 11-01-2002
F004 CLGETTS
F016 A36-002
F007 A01-01
F008 T30-01
F009 T31-10
F010 1988
F011 Bacterial
F012 T32-03
F013 T33-02
F014 A03-03
F015 100-500-1000-5000-10000 ug/plate

EOB
C
B510 TO_GENETIC_IN_VIVO_TAB
F001 27
F002 1
F003 11-01-2002
F004 CLGETTS
F018 A36-005
F007 A01-01
F008 T34-12: Rat Bone Marrow
F009 T02-24
F010 T23-47
F011 T37-15: Micronucleus Aberration
F012 1988
F013 T24-04
F014 T25-11: intragastric
F017 A03-02
EOR
F001 27
F002 2
F003 29-01-2002
F004 CLGETTS
F018 A36-002
F007 A01-03
F008 T34-12: In Vivo Mammalian Bone Marrow Erythrocyte Micronucleus Assay
*   Intraperitoneal Dosing Method
F009 T02-18
F010 T23-10
F011 T37-15: OECD 474 equivalent
F012 1988
F013 T24-03
F014 T25-11: Intraperitoneal injection
F015 12, 24 and 48 hours
F016 1.96 ml/kg Single injection
F017 A03-02
EOB
C
B511 TO_CARCINOGENICITY_TAB
F001 27
F002 1
F003 21-10-1992
F004 HEDSET
EOB
C
B512 TO_REPRODUCTION_TAB
F001 27
F002 1
F003 11-01-2002
F004 CLGETTS
F037 A36-003
F007 A01-01
F008 T41-04: two generation study with teratology screen
F009 T02-24
F010 T23-46
F011 T24-03
F012 T25-02
F013 T40-05: Comparable to an OECD 416 guideline study.

F014 1975
F015 Daily - ad libitum
F016 8 weeks
F017 8 weeks
F018 2 Generations
F019 F0 Generation: 0, 0.3, 1.0, or 3.0% solutions; F1 Generation: 0, 0.3,
*   1.0, or 2.0%
F020 T27-07
F025 A02-03
F026 1
F028 T43-01
F035 A03-01
F039 T57-10: NOAEL Maternal
F040 A02-03
F041 1
F043 T43-01
EOB
C
B513 TO_DEVELOPMENTAL_TAB
F001 27
F002 1
F003 14-01-2002
F004 CLGETTS
F030 A36-003
F007 A01-01
F008 T02-24
F009 T23-42
F010 T24-01
F011 T25-08
F012 T44-03: Comparable to an OECD 414 guideline study
F013 1989
F014 20 days
F015 Gestation Days 1-19
F016 7 hr/day
F017 3500, 5000, 7000 ppm
F018 T27-07
F019 A02-03
F020 3500
F022 T43-04
F023 A02-04
F024 7000
F026 T43-04
F029 A03-03
EOR
F001 27
F002 2
F003 11-01-2002
F004 CLGETTS
F030 A36-003
F007 A01-01
F008 T02-24
F009 T23-46
F010 T24-01
F011 T25-02
F012 T44-03: Comparable to an OECD 421 guideline study.
F013 1975
F014 20 days

F015 8 Weeks premating (Males and Females) and during gestation (Females)
F016 Daily - ad libitum
F017 0, 0.3, 1.0, or 2.0% solutions
F018 T27-07
F029 A03-01
EOB
C
B515 TO_HUMAN_EXPERIENCE_TAB
F001 27
F002 1
F003 22-10-1992
F004 HEDSET
EOB
C
B514 TO_OTHER_TAB
F001 27
F002 1
F003 11-01-2002
F004 CLGETTS
F008 A36-002
F007 T45-12: Respiratory Irritation
EOB
C
B601 TEXT_TAB
F002 27
F010 1.0.1
F004 7
F005 SO
F006 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119787
EOR
F002 27
F010 1.0.1
F004 8
F005 SO
F006 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119788
EOR
F002 27
F010 1.0.1
F004 9
F005 SO
F006 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119789
EOR

F002 27
F010 1.0.1
F004 10
F005 SO
F006 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119790
EOR
F002 27
F010 1.0.1
F004 11
F005 SO
F006 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119791
EOR
F002 27
F010 1.0.1
F004 12
F005 SO
F006 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119792
EOR
F002 27
F010 1.0.1
F004 13
F005 SO
F006 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119793
EOR
F002 27
F010 1.1.1
F004 8
F005 SO
F006 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119794
EOR
F002 27
F010 1.10

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F004 1
F005 RM
F006 As the quantities of this substance placed on the EU market
**   by Union Carbide Benelux N.V. are normally sourced from the
**   manufacturing facilities of its U.S. parent company, no
**   exposure can arise within the EU from the manufacture of
**   these s
F007 As the quantities of this substance placed on the EU market
**   by Union Carbide Benelux N.V. are normally sourced from the
**   manufacturing facilities of its U.S. parent company, no
**   exposure can arise within the EU from the manufacture of
**   these substances. The comments below on exposure are
**   restricted to uses for which Union Carbide believes its
**   customers use this substance.
**
**   Major use(s): Fuel additive in lead-free gasoline.
**
**   Sources of human exposure: Very minor sporadic exposure to
**   the public via inhalation during filling of vehicles.
**   Quantitative estimates are not available.
**
**   Sources of environmental exposure: Negligible sporadic
**   exposure to the atmosphere during filling of vehicles.
**   Quantitative estimates are not available. Substance is
**   essentially oxidised to carbon dioxide and water during
**   use.
F008 HEDSET
F009 24-05-1994
F012 20
F020 119856
EOR
F002 27
F010 1.10
F004 1
F005 SO
F006 Union Carbide Benelux  Antwerpen
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F007 Union Carbide Benelux  Antwerpen
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119857
EOR
F002 27
F010 1.10
F004 2
F005 RM
F006 Continuous process. Non-direct hydratation by absorption of
**   butenes in sulfuric acid.
**   One production site.
**   Distribution pattern : from production
**       % to air    0.02
**       % to water  0.02
**       to soil     0.0
**       to sediment 0.0
F007 Continuous process. Non-direct hydratation by absorption of
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**   butenes in sulfuric acid.
**   One production site.
**   Distribution pattern : from production
**       % to air    0.02
**       % to water  0.02
**       to soil     0.0
**       to sediment 0.0
F008 HEDSET
F009 03-06-1994
F012 20
F020 119858
EOR
F002 27
F010 1.10
F004 2
F005 SO
F006 Atochem  Paris la Defense
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F007 Atochem  Paris la Defense
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119859
EOR
F002 27
F010 1.10
F004 3
F005 RM
F006 Inhalation or skin contact when loading, unloading, using
**   the product.
**   In case of accidental release, product may contaminate the
**   environment.
F007 Inhalation or skin contact when loading, unloading, using
**   the product.
**   In case of accidental release, product may contaminate the
**   environment.
F008 HEDSET
F009 23-02-1994
F012 20
F020 119860
EOR
F002 27
F010 1.10
F004 3
F005 SO
F006 SHELL FRANCE  Rueil Malmaison
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F007 SHELL FRANCE  Rueil Malmaison
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119861
EOR
F002 27
F010 1.11
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F004 1
F005 RM
F006 DISPOSAL
**
**   Recover or recycle if possible. Otherwise incineration.
**
**
**   TRANSPORT INFORMATION
**
**   UN Number: 1120
**   Class: 3
**   Packing Group: III
**   Proper Shipping Name: Secondary butyl alcohol
**
**   Sea (IMO)
**   Class: 3.3
**   Packing Group: III
**   Symbol: Flammable
F007 DISPOSAL
**
**   Recover or recycle if possible. Otherwise incineration.
**
**
**   TRANSPORT INFORMATION
**
**   UN Number: 1120
**   Class: 3
**   Packing Group: III
**   Proper Shipping Name: Secondary butyl alcohol
**
**   Sea (IMO)
**   Class: 3.3
**   Packing Group: III
**   Symbol: Flammable liquid
**   Marine Pollutant (Y/N): No
**
**   Rail/Road (RID/ADR)
**   Class: 3
**   Item: 31(c)
**   Symbol: Flammable liquid
**   Kemler Plate: 30/1120
**
**   Air (IATA/ICAO)
**   Class: 3
**   Packing Group: III
**   Symbol: Flammable liquid
F008 HEDSET
F009 03-06-1994
F012 20
F020 119795
EOR
F002 27
F010 1.11
F004 1
F005 SO
F006 Shell Nederland Chemie B.V. Hoogvliet-Rotterdam
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

F007 Shell Nederland Chemie B.V. Hoogvliet-Rotterdam
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119796
EOR
F002 27
F010 1.11
F004 2
F005 RM
F006 Disposal: Incinerate in a furnace where permitted under
**   national and local regulations.
**
**   Transport: Butan-2-ol is classified as a class 3 product
**   according the ADR/RID/IMDG/ICAO regulations.
**   Butan-2-ol is shipped in road/rail tankcars,
**   tan
F007 Disposal: Incinerate in a furnace where permitted under
**   national and local regulations.
**
**   Transport: Butan-2-ol is classified as a class 3 product
**   according the ADR/RID/IMDG/ICAO regulations.
**   Butan-2-ol is shipped in road/rail tankcars,
**   tankcontainers/ISOtanks and smaller packages (e.g. drums).
**   ¿
F008 HEDSET
F009 26-05-1994
F012 20
F020 119797
EOR
F002 27
F010 1.11
F004 2
F005 SO
F006 Union Carbide Benelux Antwerpen
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 Union Carbide Benelux Antwerpen
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119798
EOR
F002 27
F010 1.11
F004 3
F005 RM
F006 Recover or recycle if possible. Otherwise : incineration.
**   Avoid electrostatic discharge generation.
**   Earth all equipment.
**   Avoid splash filling.
**   Use a vapour recovery system.
**   Keep in a well ventilated place.
**   Avoid naked flames. Remove ignitio
F007 Recover or recycle if possible. Otherwise : incineration.
**   Avoid electrostatic discharge generation.

```
**   Earth all equipment.
**   Avoid splash filling.
**   Use a vapour recovery system.
**   Keep in a well ventilated place.
**   Avoid naked flames. Remove ignition sources.
**   Do not smoke. Avoid sparks.
F008 HEDSET
F009 20-05-1994
F012 20
F020 119799
EOR
F002 27
F010 1.11
F004 3
F005 RM
F006 Transport
**
**   UN number : 1120
**   Class : 3
**   Packing Group : III
**   Proper Shipping Name : Secondary butyl alcohol
**
**   Sea (IMO)
**   Class : 3.3
**   Marine Pollutant : No
**   Symbol : Flammable liquid
**
**   Rail/Road (ADR/RID)
**   Class : 3
**   Item : 31 c)
**   Symbol : Flammable
F007 Transport
**
**   UN number : 1120
**   Class : 3
**   Packing Group : III
**   Proper Shipping Name : Secondary butyl alcohol
**
**   Sea (IMO)
**   Class : 3.3
**   Marine Pollutant : No
**   Symbol : Flammable liquid
**
**   Rail/Road (ADR/RID)
**   Class : 3
**   Item : 31 c)
**   Symbol : Flammable liquid
**   Kemler Plate : 30/1120
**
**   Air (IATA/IACO)
**   Class : 3
**   Symbol : Flammable liquid
F008 HEDSET
F009 20-05-1994
F012 20
F020 119800
EOR
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F002 27
F010 1.11
F004 3
F005 SO
F006 SHELL FRANCE Rueil Malmaison
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 SHELL FRANCE Rueil Malmaison
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119801
EOR
F002 27
F010 1.11
F004 4
F005 RM
F006 Disposal options:
**   Recover or recycle if possible. Otherwise: incineration.
**
**   Transport classification:
**
**   UN number: 1120
**   ADR/RID:
**   class/item: 3/31 c
**   packing group: 3
**   Kemler number: 30
**   label: 3
**   Proper shipping name: sec.-butyl alcohol
**
**   ICAO:
**   c
F007 Disposal options:
**   Recover or recycle if possible. Otherwise: incineration.
**
**   Transport classification:
**
**   UN number: 1120
**   ADR/RID:
**   class/item: 3/31 c
**   packing group: 3
**   Kemler number: 30
**   label: 3
**   Proper shipping name: sec.-butyl alcohol
**
**   ICAO:
**   class: 3
**   packing group: III
**   label: flammable liquid
**   Proper shipping name: butanols
**
**   IMO/IMDG:
**   class: 3.3
**   packing group: III
**   Marine pollutant: no
**   label: flammable liquid
**   IMDG page: 3313

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**   EMS number: 3-06
**   MFAG plate: 305
F008 HEDSET
F009 30-05-1994
F012 20
F020 119802
EOR
F002 27
F010 1.11
F004 4
F005 SO
F006 Deutsche Shell Chemie GmbH  Eschborn
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F007 Deutsche Shell Chemie GmbH  Eschborn
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119803
EOR
F002 27
F010 1.2
F004 1
F005 SO
F006 Shell Nederland Chemie B.V.  Hoogvliet-Rotterdam
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F007 Shell Nederland Chemie B.V.  Hoogvliet-Rotterdam
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119804
EOR
F002 27
F010 1.2
F004 2
F005 SO
F006 Shell Nederland Chemie B.V.  Hoogvliet-Rotterdam
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F007 Shell Nederland Chemie B.V.  Hoogvliet-Rotterdam
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119805
EOR
F002 27
F010 1.2
F004 3
F005 SO
F006 Shell Nederland Chemie B.V.  Hoogvliet-Rotterdam
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F007 Shell Nederland Chemie B.V.  Hoogvliet-Rotterdam
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
```

F020 119806
EOR
F002 27
F010 1.2
F004 4
F005 SO
F006 Union Carbide Benelux Antwerpen
**   EXXON CHEMICAL, Limited Fareham, Hampshire
**   RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
**   Hamburg
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 Union Carbide Benelux Antwerpen
**   EXXON CHEMICAL, Limited Fareham, Hampshire
**   RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
**   Hamburg
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119807
EOR
F002 27
F010 1.2
F004 5
F005 SO
F006 Union Carbide Benelux Antwerpen
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 Union Carbide Benelux Antwerpen
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119808
EOR
F002 27
F010 1.2
F004 6
F005 SO
F006 Union Carbide Benelux Antwerpen
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 Union Carbide Benelux Antwerpen
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119809
EOR
F002 27
F010 1.2
F004 7
F005 SO
F006 Atochem Paris la Defense
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 Atochem Paris la Defense
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002

F012 20
F020 119810
EOR
F002 27
F010 1.2
F004 8
F005 SO
F006 SHELL FRANCE Rueil Malmaison
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 SHELL FRANCE Rueil Malmaison
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119811
EOR
F002 27
F010 1.2
F004 9
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
**   RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
**   Hamburg
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
**   RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
**   Hamburg
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119812
EOR
F002 27
F010 1.2
F004 11
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
**   RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
**   Hamburg
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
**   RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
**   Hamburg
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119813
EOR
F002 27
F010 1.2
F004 12
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
**   RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
**   Hamburg

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**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F007 EXXON CHEMICAL, Limited  Fareham, Hampshire
**   RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
**   Hamburg
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119814
EOR
F002 27
F010 1.2
F004 13
F005 SO
F006 Deutsche Shell Chemie GmbH  Eschborn
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F007 Deutsche Shell Chemie GmbH  Eschborn
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119815
EOR
F002 27
F010 1.5
F004 8
F005 SO
F006 EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F007 EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119816
EOR
F002 27
F010 1.6.1
F004 8
F005 SO
F006 EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F007 EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119817
EOR
F002 27
F010 1.6.2
F004 13
F005 SO
F006 EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F007 EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119818
EOR
F002 27
```

F010 1.6.2
F004 14
F005 SO
F006 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119819
EOR
F002 27
F010 1.6.2
F004 15
F005 SO
F006 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119820
EOR
F002 27
F010 1.7
F004 37
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F008 CLGETTS
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F010 1.7
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F006 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
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F006 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
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F005 SO
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F007 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
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F002 27
F010 1.7
F004 41
F005 SO
F006 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
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F008 CLGETTS
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F006 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
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F007 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
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F008 CLGETTS
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F007 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119832
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F002 27
F010 1.8.1
F004 2
F005 RE
F006 Dutch MAC list 1994
F007 Dutch MAC list 1994
F008 HEDSET
F009 03-06-1994
F012 20
F020 119833
EOR
F002 27
F010 1.8.1
F004 2
F005 SO
F006 Shell Nederland Chemie B.V. Hoogvliet-Rotterdam
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 Shell Nederland Chemie B.V. Hoogvliet-Rotterdam

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**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119834
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F002 27
F010 1.8.1
F004 3
F005 RE
F006 ACGIH list 1993-1994
F007 ACGIH list 1993-1994
F008 HEDSET
F009 03-06-1994
F012 20
F020 119835
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F002 27
F010 1.8.1
F004 3
F005 SO
F006 Shell Nederland Chemie B.V.  Hoogvliet-Rotterdam
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F007 Shell Nederland Chemie B.V.  Hoogvliet-Rotterdam
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119836
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F002 27
F010 1.8.1
F004 4
F005 RE
F006 1992-1993 Threshold Limit values and Biological Exposure
**   Indices ACGIH
F007 1992-1993 Threshold Limit values and Biological Exposure
**   Indices ACGIH
F008 HEDSET
F009 26-05-1994
F012 20
F020 119837
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F002 27
F010 1.8.1
F004 4
F005 SO
F006 Union Carbide Benelux  Antwerpen
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F007 Union Carbide Benelux  Antwerpen
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119838
EOR
F002 27
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F010 1.8.1
F004 5
F005 RE
F006 INRS, Valeurs limites d'exposition professionnelle aux
** substances dangereuses de l'ACGIH aux Etats-Unis et de la
** Commission MAK en Allemagne, Cah. Notes Doc. 1992, 147,
** 195-225
F007 INRS, Valeurs limites d'exposition professionnelle aux
** substances dangereuses de l'ACGIH aux Etats-Unis et de la
** Commission MAK en Allemagne, Cah. Notes Doc. 1992, 147,
** 195-225
F008 HEDSET
F009 27-04-1994
F012 20
F020 119839
EOR
F002 27
F010 1.8.1
F004 5
F005 SO
F006 Atochem Paris la Defense
** EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 Atochem Paris la Defense
** EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119840
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F002 27
F010 1.8.1
F004 6
F005 RE
F006 INRS, Valeurs limites d'exposition professionnelle aux
** substances dangereuses de l'ACGIH aux Etats-Unis et de la
** Commission MAK en Allemagne, Cah. Notes Doc. 1992, 147,
** 195-225
F007 INRS, Valeurs limites d'exposition professionnelle aux
** substances dangereuses de l'ACGIH aux Etats-Unis et de la
** Commission MAK en Allemagne, Cah. Notes Doc. 1992, 147,
** 195-225
F008 HEDSET
F009 27-04-1994
F012 20
F020 119841
EOR
F002 27
F010 1.8.1
F004 6
F005 SO
F006 Atochem Paris la Defense
** EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 Atochem Paris la Defense
** EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20

F020 119842
EOR
F002 27
F010 1.8.1
F004 7
F005 CT
F006 France
F007 France
F008 HEDSET
F009 27-04-1994
F012 20
F020 119843
EOR
F002 27
F010 1.8.1
F004 7
F005 RE
F006 INRS, Valeurs limites d'exposition professionnelle aux
** agents chimiques en France, Cah. Notes Doc. 1993, 153,
** 557-574
F007 INRS, Valeurs limites d'exposition professionnelle aux
** agents chimiques en France, Cah. Notes Doc. 1993, 153,
** 557-574
F008 HEDSET
F009 27-04-1994
F012 20
F020 119844
EOR
F002 27
F010 1.8.1
F004 7
F005 SO
F006 Atochem Paris la Defense
** EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 Atochem Paris la Defense
** EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119845
EOR
F002 27
F010 1.8.1
F004 8
F005 RE
F006 Threshold Limit Values Book 1993-1994.
F007 Threshold Limit Values Book 1993-1994.
F008 HEDSET
F009 26-05-1994
F012 20
F020 119846
EOR
F002 27
F010 1.8.1
F004 8
F005 RM
F006 Use local exhaust ventilation.

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**   Hand protection : PVC, nitrile or neoprene gloves.
**   Eye protection  : safety monogoggles.
**   Body protection : standard issue work clothes.
**                     chemicals resistant safety shoes or boots.
F007 Use local exhaust ventilation.
**   Hand protection : PVC, nitrile or neoprene gloves.
**   Eye protection  : safety monogoggles.
**   Body protection : standard issue work clothes.
**                     chemicals resistant safety shoes or boots.
F008 HEDSET
F009 26-05-1994
F012 20
F020 119847
EOR
F002 27
F010 1.8.1
F004 8
F005 SO
F006 SHELL FRANCE  Rueil Malmaison
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F007 SHELL FRANCE  Rueil Malmaison
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119848
EOR
F002 27
F010 1.8.1
F004 9
F005 SO
F006 EXXON CHEMICAL, Limited  Fareham, Hampshire
**   RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
**   Hamburg
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F007 EXXON CHEMICAL, Limited  Fareham, Hampshire
**   RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
**   Hamburg
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119849
EOR
F002 27
F010 1.8.1
F004 10
F005 SO
F006 EXXON CHEMICAL, Limited  Fareham, Hampshire
**   RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
**   Hamburg
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F007 EXXON CHEMICAL, Limited  Fareham, Hampshire
**   RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
**   Hamburg
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F008 CLGETTS
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F009 09-01-2002
F012 20
F020 119850
EOR
F002 27
F010 1.8.1
F004 11
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119851
EOR
F002 27
F010 1.8.1
F004 12
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
**   RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
**   Hamburg
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
**   RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
**   Hamburg
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119852
EOR
F002 27
F010 1.8.1
F004 13
F005 RM
F006 Substance is easily resorbed.
F007 Substance is easily resorbed.
F008 HEDSET
F009 30-05-1994
F012 20
F020 119853
EOR
F002 27
F010 1.8.1
F004 13
F005 SO
F006 Deutsche Shell Chemie GmbH Eschborn
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 Deutsche Shell Chemie GmbH Eschborn
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119854

EOR
F002 27
F010 1.8.1
F004 16
F005 SO
F006 RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
** Hamburg
** EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
** Hamburg
** EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119855
EOR
F002 27
F010 2.1
F004 1
F005 RE
F006 Karel Verschueren. 1983. Handbook of Environmental Data on Organic
* Chemicals, 2nd Edition. Karel Verschueren (ed), pp. 301-302. Van Nostrand
* Reinhold Company, New York, NY, USA.
F007 Karel Verschueren. 1983. Handbook of Environmental Data on Organic
* Chemicals, 2nd Edition. Karel Verschueren (ed), pp. 301-302. Van Nostrand
* Reinhold Company, New York, NY, USA.
F008 CLGETTS
F012 20
F020 119862
EOR
F002 27
F010 2.1
F004 1
F005 RM
F006 Information on sBA purity is not available; assumed to have used a
* commercial grade of >/= 99%.
F007 Information on sBA purity is not available; assumed to have used a
* commercial grade of >/= 99%.
F008 CLGETTS
F012 20
F020 119863
EOR
F002 27
F010 2.1
F004 1
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
** EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
** EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119864
EOR
F002 27
F010 2.1

F004 2
F005 RE
F006 Hawley's Condensed Chemical Dictionary. Lewis, R. J., Sr., ed. 13th ed.
*   New York, NY: John Wiley & Sons, Inc. 1997.
F007 Hawley's Condensed Chemical Dictionary. Lewis, R. J., Sr., ed. 13th ed.
*   New York, NY: John Wiley & Sons, Inc. 1997.
F008 CLGETTS
F012 20
F020 119865
EOR
F002 27
F010 2.1
F004 2
F005 RM
F006 Information on sBA purity is not available; assumed to have used a
*   commercial grade of >/= 99%.
F007 Information on sBA purity is not available; assumed to have used a
*   commercial grade of >/= 99%.
F008 CLGETTS
F012 20
F020 119866
EOR
F002 27
F010 2.1
F004 2
F005 SO
F006 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F007 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F008 CLGETTS
F012 20
F020 119867
EOR
F002 27
F010 2.10
F004 1
F005 RE
F006 Safety Data Sheet (sec-butanol), June 1990, ELF ATOCHEM.
F007 Safety Data Sheet (sec-butanol), June 1990, ELF ATOCHEM.
F008 HEDSET
F009 02-06-1994
F012 20
F020 119868
EOR
F002 27
F010 2.10
F004 1
F005 RM
F006 Explosive limits of vapours in air: 1.7 to 9.8% vol.
**   Information on sBA purity is not available; assumed to have used a
*   commercial grade of >/= 99%.
F007 Explosive limits of vapours in air: 1.7 to 9.8% vol.
**   Information on sBA purity is not available; assumed to have used a
*   commercial grade of >/= 99%.
F008 HEDSET
F009 02-06-1994
F012 20
F020 119869

EOR
F002 27
F010 2.10
F004 1
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119870
EOR
F002 27
F010 2.2
F004 1
F005 RM
F006 Information on sBA purity is not available; assumed to have used a
*   commercial grade of >/= 99%.
F007 Information on sBA purity is not available; assumed to have used a
*   commercial grade of >/= 99%.
F008 CLGETTS
F012 20
F020 119871
EOR
F002 27
F010 2.2
F004 1
F005 SO
F006 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EXXON CHEMICAL, Limited Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EXXON CHEMICAL, Limited Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119872
EOR
F002 27
F010 2.2
F004 2
F005 RE
F006 Ethel Browning's Toxicity and Metabolism of Industrial Solvents. Snyder,
*   R., ed. Second Edition. Volume 3 Alcohols and Esters. New York, NY:
*   Elsevier, 1992.
F007 Ethel Browning's Toxicity and Metabolism of Industrial Solvents. Snyder,
*   R., ed. Second Edition. Volume 3 Alcohols and Esters. New York, NY:
*   Elsevier, 1992.
F008 CLGETTS
F012 20
F020 119873
EOR
F002 27
F010 2.2

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F004 2
F005 RM
F006 Information on sBA purity is not available; assumed to have used a
*    commercial grade of >/= 99%.
F007 Information on sBA purity is not available; assumed to have used a
*    commercial grade of >/= 99%.
F008 CLGETTS
F012 20
F020 119874
EOR
F002 27
F010 2.2
F004 2
F005 SO
F006 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F007 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F008 CLGETTS
F012 20
F020 119875
EOR
F002 27
F010 2.3
F004 1
F005 RE
F006 EXXON CHEMICAL, Limited  Fareham, Hampshire
F007 EXXON CHEMICAL, Limited  Fareham, Hampshire
F008 CLGETTS
F012 20
F020 119876
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F002 27
F010 2.3
F004 1
F005 SO
F006 EXXON CHEMICAL, Limited  Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F007 EXXON CHEMICAL, Limited  Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119877
EOR
F002 27
F010 2.3
F004 2
F005 RE
F006 Safety Data Sheet ELF ATOCHEM June 1990¿
F007 Safety Data Sheet ELF ATOCHEM June 1990¿
F008 HEDSET
F009 02-06-1994
F012 20
F020 119878
EOR
F002 27
F010 2.3
F004 2
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F005 RM
F006 Vapour density
F007 Vapour density
F008 HEDSET
F009 02-06-1994
F012 20
F020 119879
EOR
F002 27
F010 2.3
F004 2
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
** EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
** EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119880
EOR
F002 27
F010 2.3
F004 3
F005 RE
F006 CRC Handbook of Chemistry and Physics. Lide, D. R., ed. 81st Edition,
* pp. 3-100. CRC Press LLC, Boca Raton, FL. 2000.
F007 CRC Handbook of Chemistry and Physics. Lide, D. R., ed. 81st Edition,
* pp. 3-100. CRC Press LLC, Boca Raton, FL. 2000.
F008 CLGETTS
F012 20
F020 119881
EOR
F002 27
F010 2.3
F004 3
F005 RM
F006 Information on sBA purity is not available; assumed to have used a
* commercial grade of >/= 99%.
F007 Information on sBA purity is not available; assumed to have used a
* commercial grade of >/= 99%.
F008 CLGETTS
F012 20
F020 119882
EOR
F002 27
F010 2.3
F004 3
F005 SO
F006 ExxonBiomedical Sciences, Inc., New Jersey, USA
F007 ExxonBiomedical Sciences, Inc., New Jersey, USA
F008 CLGETTS
F012 20
F020 119883
EOR
F002 27
F010 2.4

F004 1
F005 RE
F006 Karel Verschueren. 1983. Handbook of Environmental Data on Organic
* Chemicals, 2nd Edition. Karel Verschueren (ed), pp. 301-302. Van Nostrand
* Reinhold Company, New York, NY, USA.
F007 Karel Verschueren. 1983. Handbook of Environmental Data on Organic
* Chemicals, 2nd Edition. Karel Verschueren (ed), pp. 301-302. Van Nostrand
* Reinhold Company, New York, NY, USA.
F008 CLGETTS
F012 20
F020 119884
EOR
F002 27
F010 2.4
F004 1
F005 RM
F006 Information on sBA purity is not available; assumed to have used a
* commercial grade of >/= 99%.
F007 Information on sBA purity is not available; assumed to have used a
* commercial grade of >/= 99%.
F008 CLGETTS
F012 20
F020 119885
EOR
F002 27
F010 2.4
F004 1
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
** ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
** EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
** ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
** EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119886
EOR
F002 27
F010 2.5
F004 2
F005 RE
F006 Hansch, C., Leo, A., Hoekman, D. 1995. Exploring QSAR - Hydrophobic,
* Electronic, and Steric Constants. American Chemical Society, Washington,
* DC, USA.
F007 Hansch, C., Leo, A., Hoekman, D. 1995. Exploring QSAR - Hydrophobic,
* Electronic, and Steric Constants. American Chemical Society, Washington,
* DC, USA.
F008 CLGETTS
F012 20
F020 119887
EOR
F002 27
F010 2.5
F004 2
F005 RM

F006 Information on sBA purity is not available; assumed to have used a
*   commercial grade of >/= 99%.
F007 Information on sBA purity is not available; assumed to have used a
*   commercial grade of >/= 99%.
F008 CLGETTS
F012 20
F020 119888
EOR
F002 27
F010 2.5
F004 2
F005 SO
F006 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F007 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F008 CLGETTS
F012 20
F020 119889
EOR
F002 27
F010 2.6.1
F004 1
F005 RE
F006 Karel Verschueren. 1983. Handbook of Environmental Data on Organic
*   Chemicals, 2nd Edition. Karel Verschueren (ed), pp. 301-302. Van Nostrand
*   Reinhold Company, New York, NY, USA.
F007 Karel Verschueren. 1983. Handbook of Environmental Data on Organic
*   Chemicals, 2nd Edition. Karel Verschueren (ed), pp. 301-302. Van Nostrand
*   Reinhold Company, New York, NY, USA.
F008 CLGETTS
F012 20
F020 119890
EOR
F002 27
F010 2.6.1
F004 1
F005 RM
F006 Information on sBA purity is not available; assumed to have used a
*   commercial grade of >/= 99%.
F007 Information on sBA purity is not available; assumed to have used a
*   commercial grade of >/= 99%.
F008 CLGETTS
F012 20
F020 119891
EOR
F002 27
F010 2.6.1
F004 1
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20

F020 119892
EOR
F002 27
F010 2.6.1
F004 2
F005 RE
F006 Handbook of Environmental Data on Organic Chemicals, Second
** Edition. Karel Verschueren, ed., Van Nostrand Reinhold
** Company (1983), pp. 301-302.
F007 Handbook of Environmental Data on Organic Chemicals, Second
** Edition. Karel Verschueren, ed., Van Nostrand Reinhold
** Company (1983), pp. 301-302.
F008 HEDSET
F009 02-06-1994
F012 20
F020 119893
EOR
F002 27
F010 2.6.1
F004 2
F005 RM
F006 Information on sBA purity is not available; assumed to have used a
* commercial grade of >/= 99%.
F007 Information on sBA purity is not available; assumed to have used a
* commercial grade of >/= 99%.
F008 HEDSET
F012 20
F020 119894
EOR
F002 27
F010 2.6.1
F004 2
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
** ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
** EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
** ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
** EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119895
EOR
F002 27
F010 2.6.1
F004 3
F005 RE
F006 Hefter, G.T. 1984. Solub. Data Ser., 15:94-119.
F007 Hefter, G.T. 1984. Solub. Data Ser., 15:94-119.
F008 CLGETTS
F012 20
F020 119896
EOR
F002 27
F010 2.6.1
F004 3

```
F005 RM
F006 Information on sBA purity is not available; assumed to have used a
*    commercial grade of >/= 99%.
F007 Information on sBA purity is not available; assumed to have used a
*    commercial grade of >/= 99%.
F008 CLGETTS
F012 20
F020 119897
EOR
F002 27
F010 2.6.1
F004 3
F005 SO
F006 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F007 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F008 CLGETTS
F012 20
F020 119898
EOR
F002 27
F010 2.7
F004 1
F005 SO
F006 EXXON CHEMICAL, Limited  Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F007 EXXON CHEMICAL, Limited  Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119899
EOR
F002 27
F010 2.7
F004 2
F005 RE
F006 Safety Data Sheet (sec-butanol), June 1990, ELF ATOCHEM.
F007 Safety Data Sheet (sec-butanol), June 1990, ELF ATOCHEM.
F008 HEDSET
F009 02-06-1994
F012 20
F020 119900
EOR
F002 27
F010 2.7
F004 2
F005 RM
F006 Information on sBA purity is not available; assumed to have used a
*    commercial grade of >/= 99%.
F007 Information on sBA purity is not available; assumed to have used a
*    commercial grade of >/= 99%.
F008 HEDSET
F012 20
F020 119901
EOR
F002 27
F010 2.7
```

F004 2
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119902
EOR
F002 27
F010 2.8
F004 1
F005 RE
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
F008 CLGETTS
F012 20
F020 119903
EOR
F002 27
F010 2.8
F004 1
F005 RM
F006 Information on sBA purity is not available; assumed to have used a
*   commercial grade of >/= 99%.
F007 Information on sBA purity is not available; assumed to have used a
*   commercial grade of >/= 99%.
F008 CLGETTS
F012 20
F020 119904
EOR
F002 27
F010 2.8
F004 1
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119905
EOR
F002 27
F010 2.8
F004 2
F005 RE
F006 Safety Data Sheet ELF ATOCHEM June 1990
F007 Safety Data Sheet ELF ATOCHEM June 1990
F008 HEDSET

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F009 02-06-1994
F012 20
F020 119906
EOR
F002 27
F010 2.8
F004 2
F005 SO
F006 EXXON CHEMICAL, Limited  Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F007 EXXON CHEMICAL, Limited  Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119907
EOR
F002 27
F010 2.9
F004 1
F005 RE
F006 Safety Data Sheet (sec-butanol), June 1990, ELF ATOCHEM.
F007 Safety Data Sheet (sec-butanol), June 1990, ELF ATOCHEM.
F008 HEDSET
F009 02-06-1994
F012 20
F020 119908
EOR
F002 27
F010 2.9
F004 1
F005 RM
F006 Information on sBA purity is not available; assumed to have used a
*    commercial grade of >/= 99%.
F007 Information on sBA purity is not available; assumed to have used a
*    commercial grade of >/= 99%.
F008 HEDSET
F012 20
F020 119909
EOR
F002 27
F010 2.9
F004 1
F005 SO
F006 EXXON CHEMICAL, Limited  Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F007 EXXON CHEMICAL, Limited  Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119910
EOR
F002 27
F010 3.1.1
```

F004 1
F005 RE
F006 Chemcial Hazard Assessment Division, Syracuse Research Corp. 1988.
*   Syracuse, NY, USA.
F007 Chemcial Hazard Assessment Division, Syracuse Research Corp. 1988.
*   Syracuse, NY, USA.
F008 HEDSET
F009 21-10-1992
F012 20
F020 119911
EOR
F002 27
F010 3.1.1
F004 1
F005 RM
F006 2-Butanol does not contain chromophores that adsorb light at wavelengths
*   >290 nm. Therefore, direct photolysis will not occur.
F007 2-Butanol does not contain chromophores that adsorb light at wavelengths
*   >290 nm. Therefore, direct photolysis will not occur.
F008 HEDSET
F009 21-10-1992
F012 20
F020 119912
EOR
F002 27
F010 3.1.1
F004 1
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119913
EOR
F002 27
F010 3.1.1
F004 4
F005 RE
F006 Dilling, W. L. et. al. (1976). Organic Photochemistry.
**   Simulated atmospheric photodecomposition rates of methylene
**   chloride, 1,1,1-trichloroethane, trichloroethylene,
**   tetrachloroethylene, and other compounds. Env. Sci.
**   Technol. 10(4)
F007 Dilling, W. L. et. al. (1976). Organic Photochemistry.
**   Simulated atmospheric photodecomposition rates of methylene
**   chloride, 1,1,1-trichloroethane, trichloroethylene,
**   tetrachloroethylene, and other compounds. Env. Sci.
**   Technol. 10(4), 351-356.
F008 HEDSET
F009 09-05-1994
F012 20
F020 119914
EOR
F002 27

```
F010 3.1.1
F004 4
F005 RM
F006 Information on sBA purity is not available; assumed to have used a
*    commercial grade of >/= 99%.
F007 Information on sBA purity is not available; assumed to have used a
*    commercial grade of >/= 99%.
F008 HEDSET
F012 20
F020 119915
EOR
F002 27
F010 3.1.1
F004 4
F005 RM
F006 Under simulated atmospheric conditions and in the presence
**   of 5 ppm NO, the half life of 2-butanol (10 ppm) is 4 hours.
F007 Under simulated atmospheric conditions and in the presence
**   of 5 ppm NO, the half life of 2-butanol (10 ppm) is 4 hours.
F008 HEDSET
F009 09-05-1994
F012 20
F020 119916
EOR
F002 27
F010 3.1.1
F004 4
F005 SO
F006 EXXON CHEMICAL, Limited  Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F007 EXXON CHEMICAL, Limited  Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119917
EOR
F002 27
F010 3.1.1
F004 5
F005 RE
F006 Shell International Petroleum, B.V.
F007 Shell International Petroleum, B.V.
F008 CLGETTS
F012 20
F020 119918
EOR
F002 27
F010 3.1.1
F004 5
F005 RM
F006 Calculated value using draft OECD method of Atkinson (1990).
F007 Calculated value using draft OECD method of Atkinson (1990).
F008 CLGETTS
F012 20
```

F020 119919
EOR
F002 27
F010 3.1.1
F004 5
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
** ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
** EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
** ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
** EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119920
EOR
F002 27
F010 3.1.1
F004 6
F005 RE
F006 EPIWIN. 1999. Estimation Program Interface for Windows, Version 3.04.
* Syracuse Research Corporation, Syracuse, NY, USA.
F007 EPIWIN. 1999. Estimation Program Interface for Windows, Version 3.04.
* Syracuse Research Corporation, Syracuse, NY, USA.
F008 CLGETTS
F012 20
F020 119921
EOR
F002 27
F010 3.1.1
F004 6
F005 RL
F006 Rated a 2 for reliability because it is a calculated value.
F007 Rated a 2 for reliability because it is a calculated value.
F008 CLGETTS
F012 20
F020 119922
EOR
F002 27
F010 3.1.1
F004 6
F005 RM
F006 50% degradation after 1.07 days based on a 12-hr. day. The SMILES
* (Simplified Molecular Input Line Entry System) structure used with the
* model was: OC(CC)C.
F007 50% degradation after 1.07 days based on a 12-hr. day. The SMILES
* (Simplified Molecular Input Line Entry System) structure used with the
* model was: OC(CC)C.
F008 CLGETTS
F012 20
F020 119923
EOR
F002 27
F010 3.1.1
F004 6
F005 RM

```
F006 Information on sBA purity is not available; assumed to have used a
*    commercial grade of >/= 99%.
F007 Information on sBA purity is not available; assumed to have used a
*    commercial grade of >/= 99%.
F008 CLGETTS
F012 20
F020 119924
EOR
F002 27
F010 3.1.1
F004 6
F005 SO
F006 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F007 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F008 CLGETTS
F012 20
F020 119925
EOR
F002 27
F010 3.1.1
F004 7
F005 RE
F006 Edney, E.O. and Corse, E.W. 1986. Hydroxyl radical rate constant
*    intercomparison study. EPA/600/3-86/056, US EPA, Research Triangle Park,
*    NC, US.
F007 Edney, E.O. and Corse, E.W. 1986. Hydroxyl radical rate constant
*    intercomparison study. EPA/600/3-86/056, US EPA, Research Triangle Park,
*    NC, US.
F008 CLGETTS
F012 20
F020 119926
EOR
F002 27
F010 3.1.1
F004 7
F005 RM
F006 Information on sBA purity is not available; assumed to have used a
*    commercial grade of >/= 99%.
F007 Information on sBA purity is not available; assumed to have used a
*    commercial grade of >/= 99%.
F008 CLGETTS
F012 20
F020 119927
EOR
F002 27
F010 3.1.1
F004 7
F005 RM
F006 Rate constants were determined from data developed in three labs. Two
*    equations were applied to the measured data and designated the TI
*    (time-included) and TE (time-excluded) methods. Both equations are in the
*    form of a straight line equati
F007 Rate constants were determined from data developed in three labs. Two
*    equations were applied to the measured data and designated the TI
*    (time-included) and TE (time-excluded) methods. Both equations are in the
*    form of a straight line equation, y=mx+b. Least square linear regression
*    analyses were applied to the data from each experiment.
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F008 CLGETTS
F012 20
F020 119928
EOR
F002 27
F010 3.1.1
F004 7
F005 RS
F006 Hydroxyl rate constants as calculated from measured data using the
*   time-included equation:
**
**   10.30 +/- 2.48 x 10-12 cm3/molecule-sec (r2 = 0.97); @ 24C
**   11.55 +/- 1.77 x 10-12 cm3/molecule-sec (r2 = 0.99); @ 24C
**   4.01 +/- 1.38 x 10-12 cm3/mole
F007 Hydroxyl rate constants as calculated from measured data using the
*   time-included equation:
**
**   10.30 +/- 2.48 x 10-12 cm3/molecule-sec (r2 = 0.97); @ 24C
**   11.55 +/- 1.77 x 10-12 cm3/molecule-sec (r2 = 0.99); @ 24C
**   4.01 +/- 1.38 x 10-12 cm3/molecule-sec (r2 = 0.76); @ 34C
**
**   Hydroxyl rate constants as calculated from measured data using the
*   time-excluded equation:
**
**   9.40 +/- 0.87 x 10-12 cm3/molecule-sec (r2 = 0.99); @ 24C
**   7.37 +/- 1.65 x 10-12 cm3/molecule-sec (r2 = 0.99); @ 24C
**   2.71 +/- 0.20 x 10-12 cm3/molecule-sec (r2 = 0.97); @ 34C
F008 CLGETTS
F012 20
F020 119929
EOR
F002 27
F010 3.1.1
F004 7
F005 SO
F006 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EXXON CHEMICAL, Limited Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EXXON CHEMICAL, Limited Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F012 20
F020 119930
EOR
F002 27
F010 3.1.2
F004 2
F005 RE
F006 Harris, J.C. 1982. Rate of Hydrolysis. In: Handbook of Chemical Property
*   Estimation Methods. Environmental Behavior of Organic Compounds. 7, 1-48.
*   Lyman W.J., Reehl, W.F., and Rosenblatt, D.H. (eds). McGraw-Hill, New
*   York, NY, USA.
F007 Harris, J.C. 1982. Rate of Hydrolysis. In: Handbook of Chemical Property
*   Estimation Methods. Environmental Behavior of Organic Compounds. 7, 1-48.
*   Lyman W.J., Reehl, W.F., and Rosenblatt, D.H. (eds). McGraw-Hill, New
*   York, NY, USA.

F008 HEDSET
F009 15-02-1994
F012 20
F020 119931
EOR
F002 27
F010 3.1.2
F004 2
F005 RS
F006 Hydrolysis will not contribute to the transformation of sBA in aquatic
* environments. Hydrolysis of an organic chemical is the transformation
* process in which a water molecule or hydroxide ion reacts to form a new
* carbon-oxygen bond, thereb
F007 Hydrolysis will not contribute to the transformation of sBA in aquatic
* environments. Hydrolysis of an organic chemical is the transformation
* process in which a water molecule or hydroxide ion reacts to form a new
* carbon-oxygen bond, thereby changing the parent chemical. Chemicals that
* are susceptible to hydrolysis contain functional groups that can be
* displaced by a nucleophilic substitution reaction. Simple alcohols such
* as sBA are resistant to hydrolysis because they lack a functional group
* that is hydrolytically reactive.
F008 HEDSET
F009 15-02-1994
F012 20
F020 119932
EOR
F002 27
F010 3.1.2
F004 2
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
** ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
** EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
** ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
** EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119933
EOR
F002 27
F010 3.1.3
F004 1
F005 RE
F006 Lyman, W.J. (1982). Adsorption Coefficient for Soils and Sediments. In:
* Handbook of Chemical Property Estimation Methods. Environmental Behavior
* of Organic Compounds. 4,1-33. Lyman W.J., Reehl, W.F., and Rosenblatt,
* D.H. (eds). McGraw-Hill,
F007 Lyman, W.J. (1982). Adsorption Coefficient for Soils and Sediments. In:
* Handbook of Chemical Property Estimation Methods. Environmental Behavior
* of Organic Compounds. 4,1-33. Lyman W.J., Reehl, W.F., and Rosenblatt,
* D.H. (eds). McGraw-Hill, New York, NY, USA.
F008 HEDSET
F009 21-10-1992
F012 20
F020 119934

EOR
F002 27
F010 3.1.3
F004 1
F005 RE
F006 Thomas, R.G. 1982. Volatilzation from Soil. In: Handbook of Chemical
*   Property Estimation Methods. Environmental Behavior of Organic Compounds.
*   16, 1-50. Lyman W.J., Reehl, W.F., and Rosenblatt, D.H. (eds).
*   McGraw-Hill, New York, NY, USA.
F007 Thomas, R.G. 1982. Volatilzation from Soil. In: Handbook of Chemical
*   Property Estimation Methods. Environmental Behavior of Organic Compounds.
*   16, 1-50. Lyman W.J., Reehl, W.F., and Rosenblatt, D.H. (eds).
*   McGraw-Hill, New York, NY, USA.
F008 HEDSET
F009 21-10-1992
F012 20
F020 119935
EOR
F002 27
F010 3.1.3
F004 1
F005 RM
F006 If released on land, 2-butanol has the potential to leach
**   into soil. 2-Butanol also has the potential to volatilize from dry soil.
F007 If released on land, 2-butanol has the potential to leach
**   into soil. 2-Butanol also has the potential to volatilize from dry soil.
F008 HEDSET
F009 21-10-1992
F012 20
F020 119936
EOR
F002 27
F010 3.1.3
F004 1
F005 RM
F006 The estimated log Koc for 2-butanol is 0.84. Therefore,
**   2-butanol should not absorb significantly to soil or
**   sediment.
**   The Koc value was calculated using the equation in Lyman (1982): log Koc
*   = -0.55log S + 3.64 (S, water solubility, in
F007 The estimated log Koc for 2-butanol is 0.84. Therefore,
**   2-butanol should not absorb significantly to soil or
**   sediment.
**   The Koc value was calculated using the equation in Lyman (1982): log Koc
*   = -0.55log S + 3.64 (S, water solubility, in mg/L); water solubility
*   value used = 125,000 mg/L from Hahn et al. (1986)
**   [Lyman, W.J. (1982). Adsorption Coefficient for Soils and Sediments. In:
*   Handbook of Chemical Property Estimation Methods. Environmental Behavior
*   of Organic Compounds. 4,1-33. Lyman W.J., Reehl, W.F., and Rosenblatt,
*   D.H. (eds). McGraw-Hill, New York, NY, USA.]
**   [Hahn, H-D., Dämbkes, G., and Rupprich, N. (1986). Butanols. In: Gerhartz
*   W (ed), Ullmann's encyclopedia of industrial chemistry, 5th ed, vol A4,
*   benzyl alcohol to calcium sulfate. VCH, Weinheim, 463-474.]
F008 HEDSET
F009 21-10-1992
F012 20
F020 119937

EOR
F002 27
F010 3.1.3
F004 1
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119938
EOR
F002 27
F010 3.2.1
F004 1
F005 RE
F006 Lucas, S.V. 1984. GC/MS Analysis of organics in drinking water
*   concentrates and advanced treatment concentrates. Vol. 1.
*   USEPA-600/1-84-020a (NTIS).
F007 Lucas, S.V. 1984. GC/MS Analysis of organics in drinking water
*   concentrates and advanced treatment concentrates. Vol. 1.
*   USEPA-600/1-84-020a (NTIS).
F008 HEDSET
F009 21-10-1992
F012 20
F020 119939
EOR
F002 27
F010 3.2.1
F004 1
F005 RM
F006 2-Butanol was identified in drinking water from Ottumwa, IA.
F007 2-Butanol was identified in drinking water from Ottumwa, IA.
F008 HEDSET
F009 21-10-1992
F012 20
F020 119940
EOR
F002 27
F010 3.2.1
F004 1
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119941
EOR
F002 27
F010 3.2.1

F004 2
F005 RE
F006 Great Lakes Water Quality Board. 1983. Inventory of Chemical
** Substances Indentified in the Great Lakes Ecosystem. Report
** to the Great Lakes Water Quality Board, Windsor, Canada.
F007 Great Lakes Water Quality Board. 1983. Inventory of Chemical
** Substances Indentified in the Great Lakes Ecosystem. Report
** to the Great Lakes Water Quality Board, Windsor, Canada.
F008 HEDSET
F009 21-10-1992
F012 20
F020 119942
EOR
F002 27
F010 3.2.1
F004 2
F005 RM
F006 2-Butanol has been detected in the Niagara River (Lake
** Ontario basin), but not in the western basin of Lake
** Ontario.
F007 2-Butanol has been detected in the Niagara River (Lake
** Ontario basin), but not in the western basin of Lake
** Ontario.
F008 HEDSET
F009 21-10-1992
F012 20
F020 119943
EOR
F002 27
F010 3.2.1
F004 2
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
** EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
** EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119944
EOR
F002 27
F010 3.2.1
F004 3
F005 RE
F006 Shackelford, W.M. et al. 1983. Analyt. Chim. Acta, 146:15-27
* (supplemental data).
F007 Shackelford, W.M. et al. 1983. Analyt. Chim. Acta, 146:15-27
* (supplemental data).
F008 HEDSET
F009 21-10-1992
F012 20
F020 119945
EOR
F002 27
F010 3.2.1
F004 3

F005 RM
F006 In a comprehensive survey of wastewater from 4000 industrial and
*   publically owned treatment works sponsored by the Effluent Guidelines
*   Division of the U.S. EPA, 2-butanol was identified in discharges of the
*   following industrial category (po
F007 In a comprehensive survey of wastewater from 4000 industrial and
*   publically owned treatment works sponsored by the Effluent Guidelines
*   Division of the U.S. EPA, 2-butanol was identified in discharges of the
*   following industrial category (positive occurences, median concentration
*   in ppb): leather tanning (1; 46.7), petroleum refining (1; 149.3), paint
*   and ink (1; 324.7), organics and plastics (2; 35.4), pesticides
*   manufacture (1; 36.2), pharmaceuticals (1; 4.6), foundries (1; 41.0),
*   electronics (1; 19.9), mechanical products (3; 90.6), publically owned
*   treatment works (3; 12.4). The highest effluent concentration was 920.1
*   ppb in the mechanical products industry.
F008 HEDSET
F009 21-10-1992
F012 20
F020 119946
EOR
F002 27
F010 3.2.1
F004 3
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
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F007 EXXON CHEMICAL, Limited Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119947
EOR
F002 27
F010 3.2.1
F004 4
F005 RE
F006 Sawhney, B.L. and Kozloski, R.P. 1984. J. Environ. Qual. 13:349-352.
F007 Sawhney, B.L. and Kozloski, R.P. 1984. J. Environ. Qual. 13:349-352.
F008 HEDSET
F009 21-10-1992
F012 20
F020 119948
EOR
F002 27
F010 3.2.1
F004 4
F005 RM
F006 2-Butanol was found in landfill leachate from 1 of 5 sites
**   in Connecticut. The concentration in this leachate ranged
**   from 6.2 to 14.9 ppm.
F007 2-Butanol was found in landfill leachate from 1 of 5 sites
**   in Connecticut. The concentration in this leachate ranged
**   from 6.2 to 14.9 ppm.
F008 HEDSET
F009 21-10-1992
F012 20

F020 119949
EOR
F002 27
F010 3.2.1
F004 4
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119950
EOR
F002 27
F010 3.2.1
F004 5
F005 RE
F006 Juttner, F. 1986. Chemosphere, 15: 985-992.
F007 Juttner, F. 1986. Chemosphere, 15: 985-992.
F008 HEDSET
F009 21-10-1992
F012 20
F020 119951
EOR
F002 27
F010 3.2.1
F004 5
F005 RM
F006 2-Butanol was detected but not quantified in forest air in
**   the southern Black Forest of Germany.
F007 2-Butanol was detected but not quantified in forest air in
**   the southern Black Forest of Germany.
F008 HEDSET
F009 21-10-1992
F012 20
F020 119952
EOR
F002 27
F010 3.2.1
F004 5
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119953
EOR
F002 27
F010 3.2.1
F004 6
F005 RE
F006 Snider, J.R. and Dawson, G.A. 1985. J. Geophys. Res., 90:3797-3805.

F007 Snider, J.R. and Dawson, G.A. 1985. J. Geophys. Res., 90:3797-3805.
F008 HEDSET
F009 21-10-1992
F012 20
F020 119954
EOR
F002 27
F010 3.2.1
F004 6
F005 RM
F006 Low molecular weight alcohols, including 2-butanol, were not detected in
*   air or precipitation samples taken at Tucson, Arizona, and two rural
*   sites 40 km away.
F007 Low molecular weight alcohols, including 2-butanol, were not detected in
*   air or precipitation samples taken at Tucson, Arizona, and two rural
*   sites 40 km away.
F008 HEDSET
F009 21-10-1992
F012 20
F020 119955
EOR
F002 27
F010 3.2.1
F004 6
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119956
EOR
F002 27
F010 3.3.1
F004 1
F005 RE
F006 Thomas, R.G. 1982. Volatilization from Water. In: Handbook of Chemical
*   Property Estimation Methods. Environmental Behavior of Organic Compounds.
*   15, 1-34. Lyman W.J., Reehl, W.F., and Rosenblatt, D.H. (eds).
*   McGraw-Hill, New York, NY, USA.
F007 Thomas, R.G. 1982. Volatilization from Water. In: Handbook of Chemical
*   Property Estimation Methods. Environmental Behavior of Organic Compounds.
*   15, 1-34. Lyman W.J., Reehl, W.F., and Rosenblatt, D.H. (eds).
*   McGraw-Hill, New York, NY, USA.
F008 HEDSET
F009 10-05-1994
F012 20
F020 119957
EOR
F002 27
F010 3.3.1
F004 1
F005 RS
F006 On the basis of Henry's Law constant, the volatilization half-life of
*   2-butanol is estimated to be 120.2 hours in a model river with the

```
*    follwoing parameters: 1 m deep, 1 m/sec flow rate, and 3 m/sec wind speed.
F007 On the basis of Henry's Law constant, the volatilization half-life of
*    2-butanol is estimated to be 120.2 hours in a model river with the
*    follwoing parameters: 1 m deep, 1 m/sec flow rate, and 3 m/sec wind speed.
F008 HEDSET
F009 10-05-1994
F012 20
F020 119958
EOR
F002 27
F010 3.3.1
F004 1
F005 SO
F006 EXXON CHEMICAL, Limited  Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F007 EXXON CHEMICAL, Limited  Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119959
EOR
F002 27
F010 3.3.2
F004 1
F005 RE
F006 Mackay, D. 1998. Level I Fugacity-Based Environmental Equilibrium
*    Partitioning Model, Version 2.1 (16-bit). Environmental Modelling Centre,
*    Trent University, Ontario, Canada.
F007 Mackay, D. 1998. Level I Fugacity-Based Environmental Equilibrium
*    Partitioning Model, Version 2.1 (16-bit). Environmental Modelling Centre,
*    Trent University, Ontario, Canada.
F008 HEDSET
F009 10-05-1994
F012 20
F020 119960
EOR
F002 27
F010 3.3.2
F004 1
F005 RL
F006 Rated 2 for reliability due to calculated value.
F007 Rated 2 for reliability due to calculated value.
F008 HEDSET
F012 20
F020 119961
EOR
F002 27
F010 3.3.2
F004 1
F005 RM
F006 Physicochemical data used in the calculation:
**
**   Parameter             Value w/ Units
**
```

```
**   Molecular Weight      74.12
**   Temperature           20 C
**   Log Kow               0.61
**   Water Solubility      125,000 g/m3
**   Vapor Pressure        1600 Pa
**   Melting
F007 Physicochemical data used in the calculation:
**
**   Parameter             Value w/ Units
**
**   Molecular Weight      74.12
**   Temperature           20 C
**   Log Kow               0.61
**   Water Solubility      125,000 g/m3
**   Vapor Pressure        1600 Pa
**   Melting Point         -114 C
F008 HEDSET
F009 10-05-1994
F012 20
F020 119962
EOR
F002 27
F010 3.3.2
F004 1
F005 RS
F006 Using the Mackay Level I calculation, the following
**   distribution is predicted for 2-butanol:
**
**   %Distribution    Compartment
**
**     16.28             Air
**     83.68             Water
**      0.03             Soil
**      0.01             Sediment
**      0.00
F007 Using the Mackay Level I calculation, the following
**   distribution is predicted for 2-butanol:
**
**   %Distribution    Compartment
**
**     16.28             Air
**     83.68             Water
**      0.03             Soil
**      0.01             Sediment
**      0.00             Suspended Sediment
**      0.00             Biota
F008 HEDSET
F012 20
F020 119963
EOR
F002 27
F010 3.3.2
F004 1
F005 SO
F006 EXXON CHEMICAL, Limited  Fareham, Hampshire
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F007 EXXON CHEMICAL, Limited Fareham, Hampshire
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F008 CLGETTS
F009 09-01-2002
F012 20
F020 119964
EOR
F002 27
F010 3.5
F004 2
F005 RE
F006 Sasaki, S. 1978. pp 283-298 in Aquatic Pollutants: Transfer
**   and biological effects. Hutzinger, O. et. al. (eds.)
**   Pergamon Press.
F007 Sasaki, S. 1978. pp 283-298 in Aquatic Pollutants: Transfer
**   and biological effects. Hutzinger, O. et. al. (eds.)
**   Pergamon Press.
F008 HEDSET
F009 15-02-1994
F012 20
F020 119965
EOR
F002 27
F010 3.5
F004 2
F005 RM
F006 98% BOD reduction after 5 days
F007 98% BOD reduction after 5 days
F008 HEDSET
F009 15-02-1994
F012 20
F020 119966
EOR
F002 27
F010 3.5
F004 2
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
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F007 EXXON CHEMICAL, Limited Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119967
EOR
F002 27
F010 3.5
F004 3
F005 RE
F006 Yonezawa, Y. and Urushigawa, Y. 1979. Chemosphere 8,
**   139-142.
F007 Yonezawa, Y. and Urushigawa, Y. 1979. Chemosphere 8,
**   139-142.
F008 HEDSET
F009 15-02-1994

F012 20
F020 119968
EOR
F002 27
F010 3.5
F004 3
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119969
EOR
F002 27
F010 3.5
F004 4
F005 RE
F006 Chou, W.L. et.al. 1979. Bio. Eng. Symp. 8, 391-414.
F007 Chou, W.L. et.al. 1979. Bio. Eng. Symp. 8, 391-414.
F008 HEDSET
F009 15-02-1994
F012 20
F020 119970
EOR
F002 27
F010 3.5
F004 4
F005 RM
F006 In a long-term study using anaerobic upflow filters, 93%
**   utilization rate was seen after a 52 day operation.
F007 In a long-term study using anaerobic upflow filters, 93%
**   utilization rate was seen after a 52 day operation.
F008 HEDSET
F009 15-02-1994
F012 20
F020 119971
EOR
F002 27
F010 3.5
F004 4
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119972
EOR
F002 27
F010 3.5
F004 5
F005 RE

F006 Dore et al. 1975. Trib. Cebedeau, 27:3-11.
F007 Dore et al. 1975. Trib. Cebedeau, 27:3-11.
F008 HEDSET
F009 10-05-1994
F012 20
F020 119973
EOR
F002 27
F010 3.5
F004 5
F005 RM
F006 Information on sBA purity is not available; assumed to have used a
*   commercial grade of >/= 99%.
F007 Information on sBA purity is not available; assumed to have used a
*   commercial grade of >/= 99%.
F008 HEDSET
F012 20
F020 119974
EOR
F002 27
F010 3.5
F004 5
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
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F007 EXXON CHEMICAL, Limited Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119975
EOR
F002 27
F010 3.5
F004 7
F005 RE
F006 Wagner. 1974. Wasser, 42:271-305.
F007 Wagner. 1974. Wasser, 42:271-305.
F008 HEDSET
F009 10-05-1994
F012 20
F020 119976
EOR
F002 27
F010 3.5
F004 7
F005 RM
F006 Information on sBA purity is not available; assumed to have used a
*   commercial grade of >/= 99%.
F007 Information on sBA purity is not available; assumed to have used a
*   commercial grade of >/= 99%.
F008 HEDSET
F012 20
F020 119977
EOR

F002 27
F010 3.5
F004 7
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
** ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
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F007 EXXON CHEMICAL, Limited Fareham, Hampshire
** ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
** EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119978
EOR
F002 27
F010 3.5
F004 8
F005 RE
F006 Gerhold and Malaney. 1966. J. Water Pollution Control Fed., 38:562-579.
F007 Gerhold and Malaney. 1966. J. Water Pollution Control Fed., 38:562-579.
F008 HEDSET
F009 10-05-1994
F012 20
F020 119979
EOR
F002 27
F010 3.5
F004 8
F005 RM
F006 Information on sBA purity is not available; assumed to have used a
* commercial grade of >/= 99%.
F007 Information on sBA purity is not available; assumed to have used a
* commercial grade of >/= 99%.
F008 HEDSET
F012 20
F020 119980
EOR
F002 27
F010 3.5
F004 8
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
** ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
** EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
** ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
** EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119981
EOR
F002 27
F010 3.5
F004 9
F005 RE

F006 Pitter. 1976. Water Research, 10:231-235.
F007 Pitter. 1976. Water Research, 10:231-235.
F008 HEDSET
F009 10-05-1994
F012 20
F020 119982
EOR
F002 27
F010 3.5
F004 9
F005 RM
F006 Information on sBA purity is not available; assumed to have used a
* commercial grade of >/= 99%.
F007 Information on sBA purity is not available; assumed to have used a
* commercial grade of >/= 99%.
F008 HEDSET
F012 20
F020 119983
EOR
F002 27
F010 3.5
F004 9
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
** ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
** EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
** ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
** EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 119984
EOR
F002 27
F010 3.5
F004 10
F005 ME
F006 The APHA No. 219 test method, which measures dissolved oxygen, is similar
* to the OECD 301D, Closed Bottle biodegradation test procedure.
F007 The APHA No. 219 test method, which measures dissolved oxygen, is similar
* to the OECD 301D, Closed Bottle biodegradation test procedure.
F008 CLGETTS
F012 20
F020 119985
EOR
F002 27
F010 3.5
F004 10
F005 RE
F006 Bridie, A.L., C.J.M. Wolff, and M. Winter. 1979. BOD and COD of Some
* Petrochemicals. Water Research. 13:627-630.
F007 Bridie, A.L., C.J.M. Wolff, and M. Winter. 1979. BOD and COD of Some
* Petrochemicals. Water Research. 13:627-630.
F008 CLGETTS
F012 20
F020 119986

EOR
F002 27
F010 3.5
F004 10
F005 RL
F006 Although it was cited that a standard method was followed, there is
*   little information in the article confirming that the test was conducted
*   according to the method description. This lack of information supports a
*   reliability rating of 2.
F007 Although it was cited that a standard method was followed, there is
*   little information in the article confirming that the test was conducted
*   according to the method description. This lack of information supports a
*   reliability rating of 2.
F008 CLGETTS
F012 20
F020 119987
EOR
F002 27
F010 3.5
F004 10
F005 RM
F006 Information on sBA purity is not available; assumed to have used a
*   commercial grade of >/= 99%.
F007 Information on sBA purity is not available; assumed to have used a
*   commercial grade of >/= 99%.
F008 CLGETTS
F012 20
F020 119988
EOR
F002 27
F010 3.5
F004 10
F005 RS
F006 The ThOD (theoretical oxygen demand) = 2.59 g/g. The measured BOD
*   (biological oxygen demand) = 2.15 g/g.
**   The only deviation to the test method was that 0.5 mg/L of allylthiourea
*   was added to the test medium to prevent nitrification.
F007 The ThOD (theoretical oxygen demand) = 2.59 g/g. The measured BOD
*   (biological oxygen demand) = 2.15 g/g.
**   The only deviation to the test method was that 0.5 mg/L of allylthiourea
*   was added to the test medium to prevent nitrification.
F008 CLGETTS
F012 20
F020 119989
EOR
F002 27
F010 3.5
F004 10
F005 SO
F006 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F007 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F008 CLGETTS
F012 20
F020 119990
EOR
F002 27
F010 3.5

F004 10
F005 TC
F006 10 ml of filtered wastewater was used as an inoculum with 500 ml of test
* medium. The source of the inoculum from within the wastewater treatment
* plant was not stated. The inoculum was not acclimated. There was no
* information on controls and
F007 10 ml of filtered wastewater was used as an inoculum with 500 ml of test
* medium. The source of the inoculum from within the wastewater treatment
* plant was not stated. The inoculum was not acclimated. There was no
* information on controls and replicate test samples.
** Test temperature was 20 +/- 1 deg C.
F008 CLGETTS
F012 20
F020 119991
EOR
F002 27
F010 3.5
F004 11
F005 ME
F006 The Winkler method, which measures dissolved oxygen, is equivalent to the
* OECD 301D, Closed Bottle biodegradation test procedure.
F007 The Winkler method, which measures dissolved oxygen, is equivalent to the
* OECD 301D, Closed Bottle biodegradation test procedure.
F008 CLGETTS
F012 20
F020 119992
EOR
F002 27
F010 3.5
F004 11
F005 RE
F006 Lamb, C.B. and G.F. Jenkins. 1953. B.O.D. of Synthetic Organic Chemicals.
* Procedings of the 7th Industrial Waste Conference. pp. 326-339.
F007 Lamb, C.B. and G.F. Jenkins. 1953. B.O.D. of Synthetic Organic Chemicals.
* Procedings of the 7th Industrial Waste Conference. pp. 326-339.
F008 CLGETTS
F012 20
F020 119993
EOR
F002 27
F010 3.5
F004 11
F005 RL
F006 There is little information in the article describing how the study was
* conducted. This lack of information supports a reliability rating of 2.
* The results were comparable to reported data (Bridie, A.L., C.J.M. Wolff,
* and M. Winter. 1979. B
F007 There is little information in the article describing how the study was
* conducted. This lack of information supports a reliability rating of 2.
* The results were comparable to reported data (Bridie, A.L., C.J.M. Wolff,
* and M. Winter. 1979. BOD and COD of Some Petrochemicals. Water Research.
* 13:627-630), which supports the acceptability of this study.
F008 CLGETTS
F012 20
F020 119994
EOR
F002 27

```
F010 3.5
F004 11
F005 RM
F006 Information on sBA purity is not available; assumed to have used a
*    commercial grade of >/= 99%.
F007 Information on sBA purity is not available; assumed to have used a
*    commercial grade of >/= 99%.
F008 CLGETTS
F012 20
F020 119995
EOR
F002 27
F010 3.5
F004 11
F005 RS
F006 Day    % Biodegradation (ThOD)
**
**   5              0.0
**   10            44.2
**   15            69.2
**   20            72.3
**   30            73.2
**   40            75.4
**   50            77.0
F007 Day    % Biodegradation (ThOD)
**
**   5              0.0
**   10            44.2
**   15            69.2
**   20            72.3
**   30            73.2
**   40            75.4
**   50            77.0
F008 CLGETTS
F012 20
F020 119996
EOR
F002 27
F010 3.5
F004 11
F005 SO
F006 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F007 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F008 CLGETTS
F012 20
F020 119997
EOR
F002 27
F010 3.5
F004 11
F005 TC
F006 An azide modification of the Winkler test method was used. The source of
*    the inoculum from within the wastewater treatment plant was not stated.
*    There was no information on controls and replicate test samples. Test
*    material loading was 2.5
F007 An azide modification of the Winkler test method was used. The source of
*    the inoculum from within the wastewater treatment plant was not stated.
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*    There was no information on controls and replicate test samples. Test
*    material loading was 2.5 ppm.
**   Test temperature was 20 deg C.
F008 CLGETTS
F012 20
F020 119998
EOR
F002 27
F010 3.6
F004 1
F005 RE
F006 Karel Verschueren. 1983. Handbook of Environmental Data on Organic
*    Chemicals, 2nd Edition. Karel Verschueren (ed), pp. 301-302. Van Nostrand
*    Reinhold Company, New York, NY, USA.
F007 Karel Verschueren. 1983. Handbook of Environmental Data on Organic
*    Chemicals, 2nd Edition. Karel Verschueren (ed), pp. 301-302. Van Nostrand
*    Reinhold Company, New York, NY, USA.
F008 HEDSET
F009 22-10-1992
F012 20
F020 119999
EOR
F002 27
F010 3.6
F004 1
F005 RM
F006 Information on sBA purity is not available; assumed to have used a
*    commercial grade of >/= 99%.
F007 Information on sBA purity is not available; assumed to have used a
*    commercial grade of >/= 99%.
F008 HEDSET
F012 20
F020 120000
EOR
F002 27
F010 3.6
F004 1
F005 SO
F006 EXXON CHEMICAL, Limited  Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F007 EXXON CHEMICAL, Limited  Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 120001
EOR
F002 27
F010 3.7
F004 1
F005 RE
F006 Bysshe, S.E. 1982. Biconcentration Factor in Aquatic Organisms. In:
*    Handbook of Chemical Property Estimation Methods. Environmental Behavior
*    of Organic Compounds. 5, 1-43. Lyman W.J., Reehl, W.F., and Rosenblatt,
*    D.H. (eds). McGraw-Hill, Ne
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F007 Bysshe, S.E. 1982. Biconcentration Factor in Aquatic Organisms. In:
*   Handbook of Chemical Property Estimation Methods. Environmental Behavior
*   of Organic Compounds. 5, 1-43. Lyman W.J., Reehl, W.F., and Rosenblatt,
*   D.H. (eds). McGraw-Hill, New York, NY, USA.
F008 HEDSET
F009 21-10-1992
F012 20
F020 120002
EOR
F002 27
F010 3.7
F004 1
F005 RM
F006 A bioconcentration factor of 1.7 is calculated using a 2-butanol log
*   octanol/water partition coefficient (Kow) of 0.61 as reported by Hansch
*   et al., 1995 (Hansch, C., Leo, A., Hoekman, D. 1995. Exploring QSAR -
*   Hydrophobic, Electronic, and
F007 A bioconcentration factor of 1.7 is calculated using a 2-butanol log
*   octanol/water partition coefficient (Kow) of 0.61 as reported by Hansch
*   et al., 1995 (Hansch, C., Leo, A., Hoekman, D. 1995. Exploring QSAR -
*   Hydrophobic, Electronic, and Steric Constants. American Chemical Society,
*   Washington, DC, USA.).
F008 HEDSET
F009 21-10-1992
F012 20
F020 120003
EOR
F002 27
F010 3.7
F004 1
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 120004
EOR
F002 27
F010 3.8
F004 1
F005 RE
F006 Thomas, R.G. 1982. Volatilization from Water. In: Handbook of Chemical
*   Property Estimation Methods. Environmental Behavior of Organic Compounds.
*   15, 1-34. Lyman W.J., Reehl, W.F., and Rosenblatt, D.H. (eds).
*   McGraw-Hill, New York, NY, USA.
F007 Thomas, R.G. 1982. Volatilization from Water. In: Handbook of Chemical
*   Property Estimation Methods. Environmental Behavior of Organic Compounds.
*   15, 1-34. Lyman W.J., Reehl, W.F., and Rosenblatt, D.H. (eds).
*   McGraw-Hill, New York, NY, USA.
F008 CLGETTS
F012 20
F020 120005

EOR
F002 27
F010 3.8
F004 1
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F012 20
F020 120006
EOR
F002 27
F010 4.1
F004 3
F005 RE
F006 Juhnke, I. and Luedemann, D. 1978. Results of the investigation of 200
*   chemical compounds for acute fish
**   toxicity with the golden orfe test. Z. Wasser. Abwasser
**   Forsch., 11(5):161-164.
F007 Juhnke, I. and Luedemann, D. 1978. Results of the investigation of 200
*   chemical compounds for acute fish
**   toxicity with the golden orfe test. Z. Wasser. Abwasser
**   Forsch., 11(5):161-164.
F008 HEDSET
F009 21-10-1992
F012 20
F020 120007
EOR
F002 27
F010 4.1
F004 3
F005 RM
F006 Information on sBA purity is not available; assumed to have used a
*   commercial grade of >/= 99%.
F007 Information on sBA purity is not available; assumed to have used a
*   commercial grade of >/= 99%.
F008 HEDSET
F012 20
F020 120008
EOR
F002 27
F010 4.1
F004 3
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20

F020 120009
EOR
F002 27
F010 4.1
F004 4
F005 ME
F006 Water used in the study came from Hammond Bay of Lake Huron and taken
*   from a point source that was located 250 feet offshore at a depth of
*   approximately nine feet. Test systems were 10L glass jars that contained
*   5L of lake water. Test syste
F007 Water used in the study came from Hammond Bay of Lake Huron and taken
*   from a point source that was located 250 feet offshore at a depth of
*   approximately nine feet. Test systems were 10L glass jars that contained
*   5L of lake water. Test systems were aerated. Up to six organisms were
*   added to each test system. Larval lampreys (Petromyzon marinus) were
*   collected by means of an electric shocker in the Ocqueoc River, Presque
*   Isle County, Michigan, USA, and were held in running water in aquaria and
*   samll "races" under conditions which simulated their natrual stream
*   habitat.
**
**   Water pH ranged from 7.5 to 8.2; water temperature was 55+/-1 degrees F;
*   dissolved oxygen ranged from 8.6 to 13.7 ppm; and free CO2 ranged from
*   5.0 to 9.0 ppm. Treatment solutions used were 5.0, 1.0, and 0.1 ppm. A
*   control system that only contained lake water was included. It was not
*   stated whether the units were presented as a volume or weight.
F008 CLGETTS
F012 20
F020 120010
EOR
F002 27
F010 4.1
F004 4
F005 RE
F006 Applegate, V.C. et al. 1957. Toxicity of 4,346 chemicals to larval
*   lampreys and fishes. Special Scientific Report--Fisheries No. 207. US
*   Dept. of the Interior, US Fish and Wildlife Service, Washington, DC, USA.
F007 Applegate, V.C. et al. 1957. Toxicity of 4,346 chemicals to larval
*   lampreys and fishes. Special Scientific Report--Fisheries No. 207. US
*   Dept. of the Interior, US Fish and Wildlife Service, Washington, DC, USA.
F008 HEDSET
F009 21-10-1992
F012 20
F020 120011
EOR
F002 27
F010 4.1
F004 4
F005 RM
F006 Information on sBA purity is not available; assumed to have used a
*   commercial grade of >/= 99%.
F007 Information on sBA purity is not available; assumed to have used a
*   commercial grade of >/= 99%.
F008 HEDSET
F012 20
F020 120012
EOR
F002 27

```
F010 4.1
F004 4
F005 RS
F006 The highest treatment level tested was 5 ppm. No effects were observed at
*    this level to laral lamprey.
F007 The highest treatment level tested was 5 ppm. No effects were observed at
*    this level to laral lamprey.
F008 HEDSET
F012 20
F020 120013
EOR
F002 27
F010 4.1
F004 4
F005 SO
F006 EXXON CHEMICAL, Limited  Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F007 EXXON CHEMICAL, Limited  Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 120014
EOR
F002 27
F010 4.1
F004 5
F005 ME
F006 The test method used in this study is similar to the OECD 203 test
*    guideline.
F007 The test method used in this study is similar to the OECD 203 test
*    guideline.
F008 CLGETTS
F012 20
F020 120015
EOR
F002 27
F010 4.1
F004 5
F005 ME
F006 Trimmed Spearman-Karber Method (Hamilton, M.A., R.C. Russo, and R.V.
*    Thurston. 1977. Trimmed Spearman-Karber Method for Estimating Median
*    Lethal Concentrations in Toxicity Bioassays. Environ. Sci. Technol.
*    11:714-719. Correction, 12:417, 19
F007 Trimmed Spearman-Karber Method (Hamilton, M.A., R.C. Russo, and R.V.
*    Thurston. 1977. Trimmed Spearman-Karber Method for Estimating Median
*    Lethal Concentrations in Toxicity Bioassays. Environ. Sci. Technol.
*    11:714-719. Correction, 12:417, 1978.)
F008 CLGETTS
F012 20
F020 120016
EOR
F002 27
F010 4.1
F004 5
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F005 RE
F006 Geiger D.L. et al. 1986. Acute Toxicities of Organic Chemicals to Fathead
*    Minnows (Pimephales promelas), Vol. 3. Center for Lake Superior
*    Environmental Studies. University of Wisconsin-Superior, WS, USA.
F007 Geiger D.L. et al. 1986. Acute Toxicities of Organic Chemicals to Fathead
*    Minnows (Pimephales promelas), Vol. 3. Center for Lake Superior
*    Environmental Studies. University of Wisconsin-Superior, WS, USA.
F008 CLGETTS
F012 20
F020 120017
EOR
F002 27
F010 4.1
F004 5
F005 RM
F006 Purity:  99%
F007 Purity:  99%
F008 CLGETTS
F012 20
F020 120018
EOR
F002 27
F010 4.1
F004 5
F005 RS
F006 96-hour LC50 = 3,670 mg/L (95% CI 3,380 to 3,990) based upon average,
*    corrected measured values
**   Analytical method used was Gas-Liquid Chromatography
**   Measured              Fish Total
**   Conc. (mg/L)      Mortality (@96 hrs)*
**     Control
F007 96-hour LC50 = 3,670 mg/L (95% CI 3,380 to 3,990) based upon average,
*    corrected measured values
**   Analytical method used was Gas-Liquid Chromatography
**   Measured              Fish Total
**   Conc. (mg/L)      Mortality (@96 hrs)*
**     Control                 0
**      1,018                  0
**      1,839                  0
**      2,630                  0
**      4,258                 16
**      6,667                 20
**
**   * 20 fish added at test initiation
F008 CLGETTS
F012 20
F020 120019
EOR
F002 27
F010 4.1
F004 5
F005 SO
F006 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F007 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F008 CLGETTS
F012 20
F020 120020
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EOR
F002 27
F010 4.1
F004 5
F005 TC
F006 Treatment solutions were prepared by diluting a 3.7 g/L stock solution.
* Nominal sBA treatment levels were 1.05, 1.61, 2.48, 3.82, 5.88mg/L, which
* measured 1.02, 1.84, 2.63, 4.26 and 6.67mg/L, respectively.
* Control/dilution water was EPA Dul
F007 Treatment solutions were prepared by diluting a 3.7 g/L stock solution.
* Nominal sBA treatment levels were 1.05, 1.61, 2.48, 3.82, 5.88mg/L, which
* measured 1.02, 1.84, 2.63, 4.26 and 6.67mg/L, respectively.
* Control/dilution water was EPA Duluth laboratory water. Twenty fish were
* tested per treatment and control. Tank volume = 2L. Control and treatment
* solution flow rate was equivalent to 18 chamber volumes per day.
** Mean test parameters were as follows: temperature = 24.4 deg. C;
* dissolved oxygen = 7.5 mg/L; pH = 7.8; fish age = 30 days; fish mean wt.
* = 0.09 g; fish mean length = 18.9 mm; fish loading = 0.0.90 g/L. Organism
* supplier was U.S. EPA Environmental Research Lab, Duluth, MN, USA.
F008 CLGETTS
F012 20
F020 120021
EOR
F002 27
F010 4.1
F004 6
F005 ME
F006 Interpolation from a graph of log concentration values versus percent
* mortality (APHA, 1971).
F007 Interpolation from a graph of log concentration values versus percent
* mortality (APHA, 1971).
F008 CLGETTS
F012 20
F020 120022
EOR
F002 27
F010 4.1
F004 6
F005 RE
F006 Bridie, A.L., C.J.M. Wolff, and M. Winter. 1979. The Acute Toxicity of
* Some Petrochemicals to Goldfish. Water Research. 13:623-626.
F007 Bridie, A.L., C.J.M. Wolff, and M. Winter. 1979. The Acute Toxicity of
* Some Petrochemicals to Goldfish. Water Research. 13:623-626.
F008 CLGETTS
F012 20
F020 120023
EOR
F002 27
F010 4.1
F004 6
F005 RL
F006 It is unclear from the article as to whether the reported result is based
* on nominal or measured values. This lack of information, in conjunction
* with the absence of selected test parameters and results (i.e,, exposure
* concentrations, morta
F007 It is unclear from the article as to whether the reported result is based
* on nominal or measured values. This lack of information, in conjunction

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*    with the absence of selected test parameters and results (i.e,, exposure
*    concentrations, mortality), supports a reliability rating of 2. The
*    reported value in this study is comparable to a reported fathead minnow
*    acute value for sBA: 24-hour LC50 = ~4,000 mg/L (Geiger D.L. et al. 1986.
*    Acute Toxicities of Organic Chemicals to Fathead Minnows (Pimephales
*    promelas), Vol. 3. Center for Lake Superior Environmental Studies.
*    University of Wisconsin-Superior, WS, USA.).
F008 CLGETTS
F012 20
F020 120024
EOR
F002 27
F010 4.1
F004 6
F005 RM
F006 Information on sBA purity is not available; assumed to have used a
*    commercial grade of >/= 99%.
F007 Information on sBA purity is not available; assumed to have used a
*    commercial grade of >/= 99%.
F008 CLGETTS
F012 20
F020 120025
EOR
F002 27
F010 4.1
F004 6
F005 SO
F006 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F007 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F008 CLGETTS
F012 20
F020 120026
EOR
F002 27
F010 4.1
F004 6
F005 TC
F006 A series of treatment solutions were prepared, but their concentrations
*    were not reported. Ten fish were tested per treatment. Tank volume = 25L.
*    Treatment solutions were aerated during the test. Treatment
*    concentrations were analytically v
F007 A series of treatment solutions were prepared, but their concentrations
*    were not reported. Ten fish were tested per treatment. Tank volume = 25L.
*    Treatment solutions were aerated during the test. Treatment
*    concentrations were analytically verified at test start and termination,
*    but the method of analysis was not reported. Reported results were not
*    distinguished as being based on nominal or measured values and there is
*    no control information.
**   Test parameters were as follows: temperature = 20+/-1 deg. C; dissolved
*    oxygen did not fall below 4 mg/L; initial pH = 7.0; fish average wt.  =
*    3.3+/-1.0 g; fish average length = 6.2+/-0.7 cm.
F008 CLGETTS
F012 20
F020 120027
EOR
F002 27
F010 4.1
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F004 7
F005 RE
F006 Cash, G. and V. Nabholz.. 1999. ECOSAR Classes for Microsoft Windows,
*   ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk
*   Assessment Division. Washington, DC, USA.
F007 Cash, G. and V. Nabholz.. 1999. ECOSAR Classes for Microsoft Windows,
*   ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk
*   Assessment Division. Washington, DC, USA.
F008 CLGETTS
F012 20
F020 120028
EOR
F002 27
F010 4.1
F004 7
F005 RL
F006 Rated 2 for reliability due to calculated value.
F007 Rated 2 for reliability due to calculated value.
F008 CLGETTS
F012 20
F020 120029
EOR
F002 27
F010 4.1
F004 7
F005 RM
F006 Test Type: Acute Fish Toxicity Calculation
F007 Test Type: Acute Fish Toxicity Calculation
F008 CLGETTS
F012 20
F020 120030
EOR
F002 27
F010 4.1
F004 7
F005 SO
F006 ExxonMobil Biomedical Sciences, Inc., NJ, USA
F007 ExxonMobil Biomedical Sciences, Inc., NJ, USA
F008 CLGETTS
F012 20
F020 120031
EOR
F002 27
F010 4.1
F004 7
F005 TC
F006 A log Kow (octanol/water partition coefficient) value and a chemical
*   structure are needed to complete the calculation with this model. The log
*   Kow value used was 0.61. The SMILES (Simplified Molecular Input Line
*   Entry System) structure used
F007 A log Kow (octanol/water partition coefficient) value and a chemical
*   structure are needed to complete the calculation with this model. The log
*   Kow value used was 0.61. The SMILES (Simplified Molecular Input Line
*   Entry System) structure used with the model was: OC(CC)C. Additional
*   data calculated by the model include molecular weight , 74.12, and water
*   solubility, 8,625 mg/L (@25C).
**   The reference for log Kow is: Hansch, C., A. Leo, and D. Hoekman. 1995.

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*    Exploring QSAR - Hydrophobic, Electronic, and Steric Constants. American
*    Chemical Society. Washington, DC, USA.
F008 CLGETTS
F012 20
F020 120032
EOR
F002 27
F010 4.2
F004 1
F005 RE
F006 Bringmann, G. and Kuhn, R. 1977. Results of the damaging
**   effect of water pollutants on Daphnia magna. Z. Wasser
**   Abwasser Forsch., 10(5):161-166.
F007 Bringmann, G. and Kuhn, R. 1977. Results of the damaging
**   effect of water pollutants on Daphnia magna. Z. Wasser
**   Abwasser Forsch., 10(5):161-166.
F008 HEDSET
F009 21-10-1992
F012 20
F020 120033
EOR
F002 27
F010 4.2
F004 1
F005 RM
F006 Information on sBA purity is not available; assumed to have used a
*    commercial grade of >/= 99%.
F007 Information on sBA purity is not available; assumed to have used a
*    commercial grade of >/= 99%.
F008 HEDSET
F012 20
F020 120034
EOR
F002 27
F010 4.2
F004 1
F005 SO
F006 EXXON CHEMICAL, Limited  Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F007 EXXON CHEMICAL, Limited  Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 120035
EOR
F002 27
F010 4.2
F004 2
F005 ME
F006 None applied. The EC50 was calculated arithmetically from the
*    concentration/effect ratio.
F007 None applied. The EC50 was calculated arithmetically from the
*    concentration/effect ratio.
F008 CLGETTS
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F012 20
F020 120036
EOR
F002 27
F010 4.2
F004 2
F005 ME
F006 The test method used in this study is similar to the OECD 202 test
*    guideline.
F007 The test method used in this study is similar to the OECD 202 test
*    guideline.
F008 CLGETTS
F012 20
F020 120037
EOR
F002 27
F010 4.2
F004 2
F005 RE
F006 Kuhn, R., M. Pattard, K-D. Pernak and A. Winter. 1989. Results of the
*    Harmful Effects of Selected Water Pollutants (Anilines, Phenols,
*    Aliphatic Compounds) to Daphnia magna. Water Research. 14:495-499.
F007 Kuhn, R., M. Pattard, K-D. Pernak and A. Winter. 1989. Results of the
*    Harmful Effects of Selected Water Pollutants (Anilines, Phenols,
*    Aliphatic Compounds) to Daphnia magna. Water Research. 14:495-499.
F008 CLGETTS
F012 20
F020 120038
EOR
F002 27
F010 4.2
F004 2
F005 RL
F006 Although the method was described in the article, data were not provided
*    on the test parameters or results from individual treatment and control
*    solutions. This lack of information supports a reliability rating of 2.
F007 Although the method was described in the article, data were not provided
*    on the test parameters or results from individual treatment and control
*    solutions. This lack of information supports a reliability rating of 2.
F008 CLGETTS
F012 20
F020 120039
EOR
F002 27
F010 4.2
F004 2
F005 RM
F006 Information on sBA purity is not available; assumed to have used a
*    commercial grade of >/= 99%.
F007 Information on sBA purity is not available; assumed to have used a
*    commercial grade of >/= 99%.
F008 CLGETTS
F012 20
F020 120040
EOR
F002 27
F010 4.2
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F004 2
F005 RS
F006 48-hour EC50 = 4,227 mg/L (95% CI 1,859 to 7,143) based on nominal values
** The authors considered the test valid because fewer than 10% of the
* organisms in the control were immobile, the pH value was not below 7.0,
* and the DO was not below 4
F007 48-hour EC50 = 4,227 mg/L (95% CI 1,859 to 7,143) based on nominal values
** The authors considered the test valid because fewer than 10% of the
* organisms in the control were immobile, the pH value was not below 7.0,
* and the DO was not below 4.0 mg/L at test termination.
F008 CLGETTS
F012 20
F020 120041
EOR
F002 27
F010 4.2
F004 2
F005 SO
F006 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F007 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F008 CLGETTS
F012 20
F020 120042
EOR
F002 27
F010 4.2
F004 2
F005 TC
F006 The test procedure used daphnids 6 to 24 hours old. Organisms were not
* fed during the test. The treatment medium was defined and had a total
* hardness of 2.4 mmol/L, a calcium to magnesium ratio of 4:1, a sodium to
* potassium ratio of 10:1, a
F007 The test procedure used daphnids 6 to 24 hours old. Organisms were not
* fed during the test. The treatment medium was defined and had a total
* hardness of 2.4 mmol/L, a calcium to magnesium ratio of 4:1, a sodium to
* potassium ratio of 10:1, and an initial pH value of 8.0+/-0.2. The test
* solution temperature was 20°C.
** The test systems used 50 ml beakers. Treatment solutions and controls
* were prepared in duplicate. The organism loading rate was no less than
* one animal per 2 ml test medium. 20 organisms were tested per treatment
* and control. Treatment solutions were prepared from a stock sBA solution.
* Dissolved oxygen (DO) and pH were measured at test termination although
* specific values were not supplied for this test.
F008 CLGETTS
F012 20
F020 120043
EOR
F002 27
F010 4.2
F004 3
F005 ME
F006 Probit analysis procedure using Statistical Analysis System (SAS)
* software (SAS Institute, 1989).
F007 Probit analysis procedure using Statistical Analysis System (SAS)
* software (SAS Institute, 1989).
F008 CLGETTS
F012 20

F020 120044
EOR
F002 27
F010 4.2
F004 3
F005 RE
F006 Schultz, W. and M. Tichy. 1993. Structure-Toxicity Relationships for
*   Unsaturated Alcohols to Tetrahymena pyriformis: C5 and C6 Analogs and
*   Primary Propargylic Alcohols. Environ. Contam. and Toxicology. 51:681-688.
F007 Schultz, W. and M. Tichy. 1993. Structure-Toxicity Relationships for
*   Unsaturated Alcohols to Tetrahymena pyriformis: C5 and C6 Analogs and
*   Primary Propargylic Alcohols. Environ. Contam. and Toxicology. 51:681-688.
F008 CLGETTS
F012 20
F020 120045
EOR
F002 27
F010 4.2
F004 3
F005 RL
F006 A non-standardized method was referenced in the article. Data were not
*   provided on the test parameters or results from individual treatment and
*   control solutions. This lack of information supports a reliability rating
*   of 2.
F007 A non-standardized method was referenced in the article. Data were not
*   provided on the test parameters or results from individual treatment and
*   control solutions. This lack of information supports a reliability rating
*   of 2.
F008 CLGETTS
F012 20
F020 120046
EOR
F002 27
F010 4.2
F004 3
F005 RM
F006 Information on sBA purity is not available; assumed to have used a
*   commercial grade of >/= 99%.
F007 Information on sBA purity is not available; assumed to have used a
*   commercial grade of >/= 99%.
F008 CLGETTS
F012 20
F020 120047
EOR
F002 27
F010 4.2
F004 3
F005 RS
F006 48-hour EC50 for growth = 3,196 mg/L based on nominal values
**   Population density (growth) was measured spectrophotometrically as
*   absorbance at 540 nm.
F007 48-hour EC50 for growth = 3,196 mg/L based on nominal values
**   Population density (growth) was measured spectrophotometrically as
*   absorbance at 540 nm.
F008 CLGETTS
F012 20
F020 120048

```
EOR
F002 27
F010 4.2
F004 3
F005 SO
F006 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F007 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F008 CLGETTS
F012 20
F020 120049
EOR
F002 27
F010 4.2
F004 3
F005 TC
F006 Axenic cultures of Tetrahymena pyrifomis were used in the test. Only
*    48-hour population densities were measured. Treatment solutions and
*    controls were prepared in duplicate. Treatment solutions were prepared
*    from a stock sBA solution.
F007 Axenic cultures of Tetrahymena pyrifomis were used in the test. Only
*    48-hour population densities were measured. Treatment solutions and
*    controls were prepared in duplicate. Treatment solutions were prepared
*    from a stock sBA solution.
F008 CLGETTS
F012 20
F020 120050
EOR
F002 27
F010 4.2
F004 4
F005 RE
F006 Cash, G. and V. Nabholz.. 1999. ECOSAR Classes for Microsoft Windows,
*    ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk
*    Assessment Division. Washington, DC, USA.
F007 Cash, G. and V. Nabholz.. 1999. ECOSAR Classes for Microsoft Windows,
*    ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk
*    Assessment Division. Washington, DC, USA.
F008 CLGETTS
F012 20
F020 120051
EOR
F002 27
F010 4.2
F004 4
F005 RL
F006 Rated 2 for reliability due to calculated value.
F007 Rated 2 for reliability due to calculated value.
F008 CLGETTS
F012 20
F020 120052
EOR
F002 27
F010 4.2
F004 4
F005 RM
F006 Test Type:  Acute Daphnid Toxicity Calculation
F007 Test Type:  Acute Daphnid Toxicity Calculation
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F008 CLGETTS
F012 20
F020 120053
EOR
F002 27
F010 4.2
F004 4
F005 SO
F006 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F007 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F008 CLGETTS
F012 20
F020 120054
EOR
F002 27
F010 4.2
F004 4
F005 TC
F006 A log Kow (octanol/water partition coefficient) value and a chemical
*   structure are needed to complete the calculation with this model. The log
*   Kow value used was 0.61. The SMILES (Simplified Molecular Input Line
*   Entry System) structure used
F007 A log Kow (octanol/water partition coefficient) value and a chemical
*   structure are needed to complete the calculation with this model. The log
*   Kow value used was 0.61. The SMILES (Simplified Molecular Input Line
*   Entry System) structure used with the model was: OC(CC)C. Additional
*   data calculated by the model include molecular weight , 74.12, and water
*   solubility, 8,625 mg/L (@25C).
**   The reference for log Kow is: Hansch, C., A. Leo, and D. Hoekman. 1995.
*   Exploring QSAR - Hydrophobic, Electronic, and Steric Constants. American
*   Chemical Society. Washington, DC, USA.
F008 CLGETTS
F012 20
F020 120055
EOR
F002 27
F010 4.3
F004 2
F005 RE
F006 Bringmann, G. and Kuhn, R. 1976. Vergleichende Befunde der Schadwirkung
*   wassergefahrdender Stoffe gegen Bakterien (Pseudomonas putida) und
*   Blaualgen (Microcystis aeruginosa). Gwf-Wasser/Abwasser, Vol. 117.
F007 Bringmann, G. and Kuhn, R. 1976. Vergleichende Befunde der Schadwirkung
*   wassergefahrdender Stoffe gegen Bakterien (Pseudomonas putida) und
*   Blaualgen (Microcystis aeruginosa). Gwf-Wasser/Abwasser, Vol. 117.
F008 HEDSET
F009 16-02-1994
F012 20
F020 120056
EOR
F002 27
F010 4.3
F004 2
F005 RM
F006 Information on sBA purity is not available; assumed to have used a
*   commercial grade of >/= 99%.
F007 Information on sBA purity is not available; assumed to have used a

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*    commercial grade of >/= 99%.
F008 HEDSET
F012 20
F020 120057
EOR
F002 27
F010 4.3
F004 2
F005 SO
F006 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F007 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F008 HEDSET
F012 20
F020 120058
EOR
F002 27
F010 4.3
F004 3
F005 RE
F006 Jones, H.R. 1971. Environmental control in the organic and petrochemical
*    industries. Noyes Data Corporation.
F007 Jones, H.R. 1971. Environmental control in the organic and petrochemical
*    industries. Noyes Data Corporation.
F008 HEDSET
F009 31-03-1994
F012 20
F020 120059
EOR
F002 27
F010 4.3
F004 3
F005 RM
F006 Information on sBA purity is not available; assumed to have used a
*    commercial grade of >/= 99%.
F007 Information on sBA purity is not available; assumed to have used a
*    commercial grade of >/= 99%.
F008 HEDSET
F012 20
F020 120060
EOR
F002 27
F010 4.3
F004 3
F005 SO
F006 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F007 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F008 HEDSET
F012 20
F020 120061
EOR
F002 27
F010 4.3
F004 4
F005 ME
F006 None applied. The toxicity threshold (TT) was determined graphically by
*    plotting the highest non-toxic concentration versus its mean extinction
*    value against the lowest toxic concentration versus its mean extinction
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*    value and calculating th
F007 None applied. The toxicity threshold (TT) was determined graphically by
*    plotting the highest non-toxic concentration versus its mean extinction
*    value against the lowest toxic concentration versus its mean extinction
*    value and calculating the toxicant concentration at 3% below the no
*    effect level.
F008 HEDSET
F012 20
F020 120062
EOR
F002 27
F010 4.3
F004 4
F005 RE
F006 Bringmann, G. and R. Kuhn. 1980. Comparison of the Toxicity Thresholds of
*    Water Pollutants to Bacteria, Algae, and Protozoa in the Cell
*    Multiplication Inhibition Test. Water Research. 14:231-241.
F007 Bringmann, G. and R. Kuhn. 1980. Comparison of the Toxicity Thresholds of
*    Water Pollutants to Bacteria, Algae, and Protozoa in the Cell
*    Multiplication Inhibition Test. Water Research. 14:231-241.
F008 HEDSET
F012 20
F020 120063
EOR
F002 27
F010 4.3
F004 4
F005 RL
F006 Although a non-standardized method was described in the article, data
*    were not provided on the test parameters, replication, or results from
*    individual treatment and control solutions. This lack of information
*    supports a reliability rating
F007 Although a non-standardized method was described in the article, data
*    were not provided on the test parameters, replication, or results from
*    individual treatment and control solutions. This lack of information
*    supports a reliability rating of 2.
F008 HEDSET
F012 20
F020 120064
EOR
F002 27
F010 4.3
F004 4
F005 RM
F006 Information on sBA purity is not available; assumed to have used a
*    commercial grade of >/= 99%.
F007 Information on sBA purity is not available; assumed to have used a
*    commercial grade of >/= 99%.
F008 HEDSET
F012 20
F020 120065
EOR
F002 27
F010 4.3
F004 4
F005 RM
F006 Test Type:  Static Toxicity Test
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F007 Test Type: Static Toxicity Test
F008 HEDSET
F012 20
F020 120066
EOR
F002 27
F010 4.3
F004 4
F005 RS
F006 7-day TT (toxicity threshold) for growth = 95 mg/L based on nominal
*   values.
**   The TT value for growth is calculated by identifying the treatment level
*   that is greater or equal to 3% below the treatment level that did not
*   exhibit toxic effects
F007 7-day TT (toxicity threshold) for growth = 95 mg/L based on nominal
*   values.
**   The TT value for growth is calculated by identifying the treatment level
*   that is greater or equal to 3% below the treatment level that did not
*   exhibit toxic effects as measured by the extinction of primary light of
*   monochromatic radiation at 578 nm.
F008 HEDSET
F012 20
F020 120067
EOR
F002 27
F010 4.3
F004 4
F005 SO
F006 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F007 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F008 HEDSET
F012 20
F020 120068
EOR
F002 27
F010 4.3
F004 4
F005 TC
F006 Treatment solutions were prepared by diluting a stock sBA solution.
*   Testing was conducted in metal capped, 300 ml Erlenmeyer flasks
*   containing 50 ml of treatment solution. Treatment solutions contained
*   sBA, cells, double distilled water, a
F007 Treatment solutions were prepared by diluting a stock sBA solution.
*   Testing was conducted in metal capped, 300 ml Erlenmeyer flasks
*   containing 50 ml of treatment solution. Treatment solutions contained
*   sBA, cells, double distilled water, and a sterile, defined nutrient
*   medium. The control solution contained nutrient medium, to which sterile
*   double distilled water was added. Growth inhibition measurements were
*   only determined on day 7.
**   Cell growth was determined by using a turbidimetric procedure that
*   measured primary light extinction (monochromatic radiation at 578 nm)
*   through a cell suspension of 10 mm thickness.
F008 HEDSET
F012 20
F020 120069
EOR
F002 27

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F010 4.3
F004 5
F005 RE
F006 Cash, G. and V. Nabholz.. 1999. ECOSAR Classes for Microsoft Windows,
*    ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk
*    Assessment Division. Washington, DC, USA.
F007 Cash, G. and V. Nabholz.. 1999. ECOSAR Classes for Microsoft Windows,
*    ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk
*    Assessment Division. Washington, DC, USA.
F008 HEDSET
F012 20
F020 120070
EOR
F002 27
F010 4.3
F004 5
F005 RL
F006 Rated 2 for reliability due to calculated value.
F007 Rated 2 for reliability due to calculated value.
F008 HEDSET
F012 20
F020 120071
EOR
F002 27
F010 4.3
F004 5
F005 RM
F006 Test Type:  Green Alga Toxicity Calculation
F007 Test Type:  Green Alga Toxicity Calculation
F008 HEDSET
F012 20
F020 120072
EOR
F002 27
F010 4.3
F004 5
F005 RS
F006 96-hour EC50 = 625 mg/L
F007 96-hour EC50 = 625 mg/L
F008 HEDSET
F012 20
F020 120073
EOR
F002 27
F010 4.3
F004 5
F005 SO
F006 ExxonMobil Biomedical Sciences, Inc., NJ, USA
F007 ExxonMobil Biomedical Sciences, Inc., NJ, USA
F008 HEDSET
F012 20
F020 120074
EOR
F002 27
F010 4.3
F004 5
F005 TC
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F006 A log Kow (octanol/water partition coefficient) value and a chemical
*    structure are needed to complete the calculation with this model. The log
*    Kow value used was 0.61. The SMILES (Simplified Molecular Input Line
*    Entry System) structure used
F007 A log Kow (octanol/water partition coefficient) value and a chemical
*    structure are needed to complete the calculation with this model. The log
*    Kow value used was 0.61. The SMILES (Simplified Molecular Input Line
*    Entry System) structure used with the model was: OC(CC)C.  Additional
*    data calculated by the model include molecular weight , 74.12, and water
*    solubility, 8,625 mg/L (@25C).
**   The reference for log Kow is: Hansch, C., A. Leo, and D. Hoekman. 1995.
*    Exploring QSAR - Hydrophobic, Electronic, and Steric Constants. American
*    Chemical Society. Washington, DC, USA.
F008 HEDSET
F012 20
F020 120075
EOR
F002 27
F010 4.3
F004 6
F005 RE
F006 Cash, G. and V. Nabholz.. 1999. ECOSAR Classes for Microsoft Windows,
*    ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk
*    Assessment Division. Washington, DC, USA.
F007 Cash, G. and V. Nabholz.. 1999. ECOSAR Classes for Microsoft Windows,
*    ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk
*    Assessment Division. Washington, DC, USA.
F008 HEDSET
F012 20
F020 120076
EOR
F002 27
F010 4.3
F004 6
F005 RL
F006 Rated 2 for reliability due to calculated value.
F007 Rated 2 for reliability due to calculated value.
F008 HEDSET
F012 20
F020 120077
EOR
F002 27
F010 4.3
F004 6
F005 RS
F006 *Chronic value
F007 *Chronic value
F008 HEDSET
F012 20
F020 120078
EOR
F002 27
F010 4.3
F004 6
F005 SO
F006 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F007 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
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F008 HEDSET
F012 20
F020 120079
EOR
F002 27
F010 4.3
F004 6
F005 TC
F006 A log Kow (octanol/water partition coefficient) value and a chemical
*   structure are needed to complete the calculation with this model. The log
*   Kow value used was 0.61. The SMILES (Simplified Molecular Input Line
*   Entry System) structure used
F007 A log Kow (octanol/water partition coefficient) value and a chemical
*   structure are needed to complete the calculation with this model. The log
*   Kow value used was 0.61. The SMILES (Simplified Molecular Input Line
*   Entry System) structure used with the model was: OC(CC)C. Additional
*   data calculated by the model include molecular weight , 74.12, and water
*   solubility, 8,625 mg/L (@25C).
**   The reference for log Kow is: Hansch, C., A. Leo, and D. Hoekman. 1995.
*   Exploring QSAR - Hydrophobic, Electronic, and Steric Constants. American
*   Chemical Society. Washington, DC, USA.
F008 HEDSET
F012 20
F020 120080
EOR
F002 27
F010 4.4
F004 1
F005 RE
F006 Bringmann, G. and R. Kuhn. 1980. Comparison of the toxicity thresholds
*   of water pollutants to bacteria, algae and protozoa in the cell
*   multiplication inhibition test. Water Research, 14:231-241.
F007 Bringmann, G. and R. Kuhn. 1980. Comparison of the toxicity thresholds
*   of water pollutants to bacteria, algae and protozoa in the cell
*   multiplication inhibition test. Water Research, 14:231-241.
F008 HEDSET
F009 20-10-1992
F012 20
F020 120081
EOR
F002 27
F010 4.4
F004 1
F005 RM
F006 Information on sBA purity is not available; assumed to have used a
*   commercial grade of >/= 99%.
F007 Information on sBA purity is not available; assumed to have used a
*   commercial grade of >/= 99%.
F008 HEDSET
F012 20
F020 120082
EOR
F002 27
F010 4.4
F004 1
F005 SO
F006 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA

F007 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F008 HEDSET
F012 20
F020 120083
EOR
F002 27
F010 4.4
F004 2
F005 RE
F006 Environmental Health Criteria 65: Butanols: four isomers:
** 1-butanol, 2-butanol, tert-butanol, isobutanol. 1987. IPCS
** International Programme on Chemical Safety, World Health
** Organization.
F007 Environmental Health Criteria 65: Butanols: four isomers:
** 1-butanol, 2-butanol, tert-butanol, isobutanol. 1987. IPCS
** International Programme on Chemical Safety, World Health
** Organization.
F008 HEDSET
F009 20-10-1992
F012 20
F020 120084
EOR
F002 27
F010 4.4
F004 2
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
** ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
** EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
** ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
** EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 120085
EOR
F002 27
F010 4.4
F004 3
F005 RE
F006 Bringmann, G. and Kuhn, R. 1980. Bestimmung der biologischen Schadwirkung
* wassergefahrdender Stoffe gegen Protozoen. II. Bakterienfressende
* Ciliaten. Z. Wasser/Abwasser Forsch., 1:26-31.
F007 Bringmann, G. and Kuhn, R. 1980. Bestimmung der biologischen Schadwirkung
* wassergefahrdender Stoffe gegen Protozoen. II. Bakterienfressende
* Ciliaten. Z. Wasser/Abwasser Forsch., 1:26-31.
F008 CLGETTS
F012 20
F020 120086
EOR
F002 27
F010 4.4
F004 3
F005 RM
F006 Information on sBA purity is not available; assumed to have used a
* commercial grade of >/= 99%.

F007 Information on sBA purity is not available; assumed to have used a
*   commercial grade of >/= 99%.
F008 CLGETTS
F012 20
F020 120087
EOR
F002 27
F010 4.4
F004 3
F005 SO
F006 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F007 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F008 CLGETTS
F012 20
F020 120088
EOR
F002 27
F010 4.4
F004 4
F005 RM
F006 Information on sBA purity is not available; assumed to have used a
*   commercial grade of >/= 99%.
F007 Information on sBA purity is not available; assumed to have used a
*   commercial grade of >/= 99%.
F008 CLGETTS
F012 20
F020 120089
EOR
F002 27
F010 4.4
F004 4
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 120090
EOR
F002 27
F010 4.4
F004 5
F005 RE
F006 Bringmann, G. and Kuhn, R. 1980. Comparison of the toxicity thresholds of
*   water pollutants to bacteria, algae and protozoa in the cell
*   multiplication inhibition test. Water Research, 14:231-241.
F007 Bringmann, G. and Kuhn, R. 1980. Comparison of the toxicity thresholds of
*   water pollutants to bacteria, algae and protozoa in the cell
*   multiplication inhibition test. Water Research, 14:231-241.
F008 CLGETTS
F012 20
F020 120091
EOR

F002 27
F010 4.4
F004 5
F005 RM
F006 Information on sBA purity is not available; assumed to have used a
*   commercial grade of >/= 99%.
F007 Information on sBA purity is not available; assumed to have used a
*   commercial grade of >/= 99%.
F008 CLGETTS
F012 20
F020 120092
EOR
F002 27
F010 4.4
F004 5
F005 SO
F006 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F007 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F008 CLGETTS
F012 20
F020 120093
EOR
F002 27
F010 4.5.1
F004 1
F005 RE
F006 Cash, G. and V. Nabholz.. 1999. ECOSAR Classes for Microsoft Windows,
*   ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk
*   Assessment Division. Washington, DC, USA.
F007 Cash, G. and V. Nabholz.. 1999. ECOSAR Classes for Microsoft Windows,
*   ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk
*   Assessment Division. Washington, DC, USA.
F008 CLGETTS
F012 20
F020 120094
EOR
F002 27
F010 4.5.1
F004 1
F005 RL
F006 Rated 2 for reliability due to calculated value.
F007 Rated 2 for reliability due to calculated value.
F008 CLGETTS
F012 20
F020 120095
EOR
F002 27
F010 4.5.1
F004 1
F005 RM
F006 Test Type: Chronic Fish Toxicity Calculation
**   * Chronic Value
F007 Test Type: Chronic Fish Toxicity Calculation
**   * Chronic Value
F008 CLGETTS
F012 20
F020 120096

EOR
F002 27
F010 4.5.1
F004 1
F005 SO
F006 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F007 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F008 CLGETTS
F012 20
F020 120097
EOR
F002 27
F010 4.5.1
F004 1
F005 TC
F006 A log Kow (octanol/water partition coefficient) value and a chemical
*   structure are needed to complete the calculation with this model. The log
*   Kow value used was 0.61. The SMILES (Simplified Molecular Input Line
*   Entry System) structure used
F007 A log Kow (octanol/water partition coefficient) value and a chemical
*   structure are needed to complete the calculation with this model. The log
*   Kow value used was 0.61. The SMILES (Simplified Molecular Input Line
*   Entry System) structure used with the model was: OC(CC)C. Additional
*   data calculated by the model include molecular weight , 74.12, and water
*   solubility, 8,625 mg/L (@25C).
**   The reference for log Kow is: Hansch, C., A. Leo, and D. Hoekman. 1995.
*   Exploring QSAR - Hydrophobic, Electronic, and Steric Constants. American
*   Chemical Society. Washington, DC, USA.
F008 CLGETTS
F012 20
F020 120098
EOR
F002 27
F010 4.5.2
F004 1
F005 RE
F006 Cash, G. and V. Nabholz.. 1999. ECOSAR Classes for Microsoft Windows,
*   ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk
*   Assessment Division. Washington, DC, USA.
F007 Cash, G. and V. Nabholz.. 1999. ECOSAR Classes for Microsoft Windows,
*   ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk
*   Assessment Division. Washington, DC, USA.
F008 CLGETTS
F012 20
F020 120099
EOR
F002 27
F010 4.5.2
F004 1
F005 RL
F006 Rated 2 for reliability due to calculated value.
F007 Rated 2 for reliability due to calculated value.
F008 CLGETTS
F012 20
F020 120100
EOR
F002 27

F010 4.5.2
F004 1
F005 RM
F006 Test Type: Chronic Daphnid Toxicity Calculation
F007 Test Type: Chronic Daphnid Toxicity Calculation
F008 CLGETTS
F012 20
F020 120101
EOR
F002 27
F010 4.5.2
F004 1
F005 SO
F006 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F007 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F008 CLGETTS
F012 20
F020 120102
EOR
F002 27
F010 4.5.2
F004 1
F005 TC
F006 A log Kow (octanol/water partition coefficient) value and a chemical
*   structure are needed to complete the calculation with this model. The log
*   Kow value used was 0.61. The SMILES (Simplified Molecular Input Line
*   Entry System) structure used
F007 A log Kow (octanol/water partition coefficient) value and a chemical
*   structure are needed to complete the calculation with this model. The log
*   Kow value used was 0.61. The SMILES (Simplified Molecular Input Line
*   Entry System) structure used with the model was: OC(CC)C. Additional
*   data calculated by the model include molecular weight , 74.12, and water
*   solubility, 8,625 mg/L (@25C).
**   The reference for log Kow is: Hansch, C., A. Leo, and D. Hoekman. 1995.
*   Exploring QSAR - Hydrophobic, Electronic, and Steric Constants. American
*   Chemical Society. Washington, DC, USA.
F008 CLGETTS
F012 20
F020 120103
EOR
F002 27
F010 4.6.2
F004 1
F005 RE
F006 World Health Organization. 1987. Environmental Health Criteria 65.
F007 World Health Organization. 1987. Environmental Health Criteria 65.
F008 HEDSET
F009 20-10-1992
F012 20
F020 120109
EOR
F002 27
F010 4.6.2
F004 1
F005 RM
F006 Information on sBA purity is not available; assumed to have used a
*   commercial grade of >/= 99%.

F007 Information on sBA purity is not available; assumed to have used a
*   commercial grade of >/= 99%.
F008 HEDSET
F012 20
F020 120110
EOR
F002 27
F010 4.6.2
F004 1
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 120111
EOR
F002 27
F010 4.6.2
F004 2
F005 RE
F006 World Health Organization. 1987. Environmental Health Criteria 65.
F007 World Health Organization. 1987. Environmental Health Criteria 65.
F008 HEDSET
F009 20-10-1992
F012 20
F020 120112
EOR
F002 27
F010 4.6.2
F004 2
F005 RM
F006 Information on sBA purity is not available; assumed to have used a
*   commercial grade of >/= 99%.
F007 Information on sBA purity is not available; assumed to have used a
*   commercial grade of >/= 99%.
F008 HEDSET
F012 20
F020 120113
EOR
F002 27
F010 4.6.2
F004 2
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20

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F020 120114
EOR
F002 27
F010 4.6.2
F004 3
F005 ME
F006 Stage at application: seedling, on intact plant; addition to
**    growth meduim, in culture flask, dose = 1%.
F007 Stage at application: seedling, on intact plant; addition to
**    growth meduim, in culture flask, dose = 1%.
F008 CLGETTS
F012 20
F020 120115
EOR
F002 27
F010 4.6.2
F004 3
F005 RE
F006 Macht, D.I. and Meyer, J.D. 1933. Am. J. Botany, 20:145-149.
F007 Macht, D.I. and Meyer, J.D. 1933. Am. J. Botany, 20:145-149.
F008 HEDSET
F009 15-02-1994
F012 20
F020 120116
EOR
F002 27
F010 4.6.2
F004 3
F005 RM
F006 Information on sBA purity is not available; assumed to have used a
*    commercial grade of >/= 99%.
F007 Information on sBA purity is not available; assumed to have used a
*    commercial grade of >/= 99%.
F008 HEDSET
F012 20
F020 120117
EOR
F002 27
F010 4.6.2
F004 3
F005 RS
F006 73% size decrease of root
F007 73% size decrease of root
F008 HEDSET
F012 20
F020 120118
EOR
F002 27
F010 4.6.2
F004 3
F005 SO
F006 EXXON CHEMICAL, Limited  Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F007 EXXON CHEMICAL, Limited  Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
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F008 CLGETTS
F009 09-01-2002
F012 20
F020 120119
EOR
F002 27
F010 4.6.2
F004 4
F005 ME
F006 stage at application: seedling, on intact plant, in
** environmental chamber, application by fumigation: 2 cm3/l.
F007 stage at application: seedling, on intact plant, in
** environmental chamber, application by fumigation: 2 cm3/l.
F008 CLGETTS
F012 20
F020 120120
EOR
F002 27
F010 4.6.2
F004 4
F005 RE
F006 Miller, L.P. 1934. Contr. Boy. T., 6:279-296.
F007 Miller, L.P. 1934. Contr. Boy. T., 6:279-296.
F008 HEDSET
F009 15-02-1994
F012 20
F020 120121
EOR
F002 27
F010 4.6.2
F004 4
F005 RM
F006 Information on sBA purity is not available; assumed to have used a
* commercial grade of >/= 99%.
F007 Information on sBA purity is not available; assumed to have used a
* commercial grade of >/= 99%.
F008 HEDSET
F012 20
F020 120122
EOR
F002 27
F010 4.6.2
F004 4
F005 RS
F006 20% respiration increase, on tuber
F007 20% respiration increase, on tuber
F008 HEDSET
F012 20
F020 120123
EOR
F002 27
F010 4.6.2
F004 4
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
** ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
** EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

F007 EXXON CHEMICAL, Limited Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 120124
EOR
F002 27
F010 4.6.2
F004 5
F005 ME
F006 Stage at application: seedling, on excised organ; addition
**   to growth medium, dose: 5 x 10 E-2 M.
F007 Stage at application: seedling, on excised organ; addition
**   to growth medium, dose: 5 x 10 E-2 M.
F008 CLGETTS
F012 20
F020 120125
EOR
F002 27
F010 4.6.2
F004 5
F005 RE
F006 Gudjonsdottir, S. and Burstrom, H. 1962. Physl. Plant, 15:498-504.
F007 Gudjonsdottir, S. and Burstrom, H. 1962. Physl. Plant, 15:498-504.
F008 HEDSET
F009 15-02-1994
F012 20
F020 120126
EOR
F002 27
F010 4.6.2
F004 5
F005 RM
F006 Information on sBA purity is not available; assumed to have used a
*   commercial grade of >/= 99%.
F007 Information on sBA purity is not available; assumed to have used a
*   commercial grade of >/= 99%.
F008 HEDSET
F012 20
F020 120127
EOR
F002 27
F010 4.6.2
F004 5
F005 RS
F006 50% size decrease of cells
F007 50% size decrease of cells
F008 HEDSET
F012 20
F020 120128
EOR
F002 27
F010 4.6.2
F004 5
F005 SO

F006 EXXON CHEMICAL, Limited Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 120129
EOR
F002 27
F010 4.6.2
F004 6
F005 ME
F006 Stage at application: seedling, on excised organ; addition
**   to growth medium, dose: 4 x 10E-2 M
F007 Stage at application: seedling, on excised organ; addition
**   to growth medium, dose: 4 x 10E-2 M
F008 CLGETTS
F012 20
F020 120130
EOR
F002 27
F010 4.6.2
F004 6
F005 RE
F006 Gudjonsdottir, S. and Burstrom, H. Physl. Plant, 15:498-504.
F007 Gudjonsdottir, S. and Burstrom, H. Physl. Plant, 15:498-504.
F008 HEDSET
F009 15-02-1994
F012 20
F020 120131
EOR
F002 27
F010 4.6.2
F004 6
F005 RM
F006 Information on sBA purity is not available; assumed to have used a
*   commercial grade of >/= 99%.
F007 Information on sBA purity is not available; assumed to have used a
*   commercial grade of >/= 99%.
F008 HEDSET
F012 20
F020 120132
EOR
F002 27
F010 4.6.2
F004 6
F005 RS
F006 50% decrease in number of cells
F007 50% decrease in number of cells
F008 HEDSET
F012 20
F020 120133
EOR
F002 27

F010 4.6.2
F004 6
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
**   ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 120134
EOR
F002 27
F010 4.6.3
F004 1
F005 RE
F006 Cash, G. and V. Nabholz.. 1999. ECOSAR Classes for Microsoft Windows,
*   ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk
*   Assessment Division. Washington, DC, USA.
F007 Cash, G. and V. Nabholz.. 1999. ECOSAR Classes for Microsoft Windows,
*   ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk
*   Assessment Division. Washington, DC, USA.
F008 CLGETTS
F012 20
F020 120104
EOR
F002 27
F010 4.6.3
F004 1
F005 RL
F006 Rated 2 for reliability due to calculated value.
F007 Rated 2 for reliability due to calculated value.
F008 CLGETTS
F012 20
F020 120105
EOR
F002 27
F010 4.6.3
F004 1
F005 RM
F006 Test Type: Earthworm Toxicity Calculation
F007 Test Type: Earthworm Toxicity Calculation
F008 CLGETTS
F012 20
F020 120106
EOR
F002 27
F010 4.6.3
F004 1
F005 SO
F006 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F007 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F008 CLGETTS
F012 20
F020 120107

EOR
F002 27
F010 4.6.3
F004 1
F005 TC
F006 A log Kow (octanol/water partition coefficient) value and a chemical
*   structure are needed to complete the calculation with this model. The log
*   Kow value used was 0.61. The SMILES (Simplified Molecular Input Line
*   Entry System) structure used
F007 A log Kow (octanol/water partition coefficient) value and a chemical
*   structure are needed to complete the calculation with this model. The log
*   Kow value used was 0.61. The SMILES (Simplified Molecular Input Line
*   Entry System) structure used with the model was: OC(CC)C. Additional
*   data calculated by the model include molecular weight , 74.12, and water
*   solubility, 8,625 mg/L (@25C).
**   The reference for log Kow is: Hansch, C., A. Leo, and D. Hoekman. 1995.
*   Exploring QSAR - Hydrophobic, Electronic, and Steric Constants. American
*   Chemical Society. Washington, DC, USA.
F008 CLGETTS
F012 20
F020 120108
EOR
F002 27
F010 4.6.4
F004 2
F005 ME
F006 Median lethal concentration was calculated as a projection from the least
*   square linear regression on log transformed nominal concentration data
*   and probit transformed percent effect data.
F007 Median lethal concentration was calculated as a projection from the least
*   square linear regression on log transformed nominal concentration data
*   and probit transformed percent effect data.
F008 CLGETTS
F012 20
F020 120135
EOR
F002 27
F010 4.6.4
F004 2
F005 RE
F006 de Zwart, D. and Slooff, W. 1987. Toxicity of Mixtures of Heavy Metals
*   and Petrochemicals to Xenopus laevis. Bull. Environ. Contam. Toxicol.,
*   38:345-351.
F007 de Zwart, D. and Slooff, W. 1987. Toxicity of Mixtures of Heavy Metals
*   and Petrochemicals to Xenopus laevis. Bull. Environ. Contam. Toxicol.,
*   38:345-351.
F008 CLGETTS
F012 20
F020 120136
EOR
F002 27
F010 4.6.4
F004 2
F005 RL
F006 The test procedure was generally described in the article. Data were not
*   provided on the test parameters or results from individual treatment and
*   control solutions. This lack of information supports a reliability rating

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*    of 2.
F007 The test procedure was generally described in the article. Data were not
*    provided on the test parameters or results from individual treatment and
*    control solutions. This lack of information supports a reliability rating
*    of 2.
F008 CLGETTS
F012 20
F020 120137
EOR
F002 27
F010 4.6.4
F004 2
F005 RM
F006 Test Type:  Static Acute Toxicity Test
**   Analytical Monitoring:  No
**   Results based on nominal treatment values.
**   Information on sBA purity is not available; assumed to have used a
*    commercial grade of >/= 99%.
F007 Test Type:  Static Acute Toxicity Test
**   Analytical Monitoring:  No
**   Results based on nominal treatment values.
**   Information on sBA purity is not available; assumed to have used a
*    commercial grade of >/= 99%.
F008 CLGETTS
F012 20
F020 120138
EOR
F002 27
F010 4.6.4
F004 2
F005 SO
F006 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F007 ExxonMobil Biomedical Sciences, Inc., New Jersey, USA
F008 CLGETTS
F012 20
F020 120139
EOR
F002 27
F010 4.6.4
F004 2
F005 TC
F006 The test procedure used 3 to 4 week old larvae. The organisms were
*    exposed in covered all-glass aquaria containing 1L of Dutch Standard
*    Water at a temperature of 20+/-1C. The test material was added once at
*    the beginning of the study. Five
F007 The test procedure used 3 to 4 week old larvae. The organisms were
*    exposed in covered all-glass aquaria containing 1L of Dutch Standard
*    Water at a temperature of 20+/-1C. The test material was added once at
*    the beginning of the study. Five concentration levels were evaluated with
*    10 organisms per level. The 5 levels had a factorial difference of 1.5.
*    Mortality was only recorded after 48 hours.
**   The test species, Xenopus laevis, was identified in the article as a
*    clawed toad. However, it is correctly identified as a clawed frog in this
*    robust summary.
F008 CLGETTS
F012 20
F020 120140
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EOR
F002 27
F010 5.0
F004 1
F005 CL
F006 In the development of the model, the authors confirmed that a limited
*   amount of sBA could be recovered as glucuronide in the urine. Most of the
*   alcohol appears to undergo oxidation via alcohol dehydrogenase to its
*   corresponding ketone, MEK.
F007 In the development of the model, the authors confirmed that a limited
*   amount of sBA could be recovered as glucuronide in the urine. Most of the
*   alcohol appears to undergo oxidation via alcohol dehydrogenase to its
*   corresponding ketone, MEK. The results showed a limited amount of the
*   ketone undergoes a backward reduction to its parent alcohol, sBA. 3H-2B
*   and 2,3-BD are found to be common metabolites of sBA and MEK. The model
*   was able to simulate blood concentrations and elimination of all 4
*   compounds after oral administration of sBA, and the results after i.v. of
*   3H-2B and 2,3-BD. AUC analysis suggested that the quantities of 3H-2B
*   and 2,3-BD formed from oral doses of sBA and MEK are comparable. The
*   results supported the estimation in that no significant difference in the
*   AUC of MEK was observed after dosing with either 1776 mg/kg of sBA or
*   1690 mg/kg of MEK (10,899 ± 824 vs. 9868 ± 566 mg-hr /liter,
*   respectively).
F020 255640
EOR
F002 27
F010 5.0
F004 1
F005 ME
F006 Statistical Methods
**   Student's t-test was used for statistical evaluation of differences
*   between two means. In the pharmacokinetic model, the differential
*   equations were solved numerically by a Hammings Predictor-Correction
*   method with a Ru
F007 Statistical Methods
**   Student's t-test was used for statistical evaluation of differences
*   between two means. In the pharmacokinetic model, the differential
*   equations were solved numerically by a Hammings Predictor-Correction
*   method with a Runge-Kutta starter.
F020 255637
EOR
F002 27
F010 5.0
F004 1
F005 RE
F006 Dietz FK, Rodrigues-Giaxola M, Traiger GJ, Stella VJ and Himmelstein KJ
*   (1981). Pharmacokinetics of 2-Butanol and its metabolites in the rat.
*   Journal of Pharmacokinetics and Biopharmaceutics 9(5), 553-576.
F007 Dietz FK, Rodrigues-Giaxola M, Traiger GJ, Stella VJ and Himmelstein KJ
*   (1981). Pharmacokinetics of 2-Butanol and its metabolites in the rat.
*   Journal of Pharmacokinetics and Biopharmaceutics 9(5), 553-576.
F020 255642
EOR
F002 27
F010 5.0
F004 1
F005 RL

F006 No circumstances occurred that would have affected the quality or
*   integrity of the data. Test procedures were in accordance with generally
*   accepted scientific standards and described in sufficient detail.
F007 No circumstances occurred that would have affected the quality or
*   integrity of the data. Test procedures were in accordance with generally
*   accepted scientific standards and described in sufficient detail.
F020 255641
EOR
F002 27
F010 5.0
F004 1
F005 RM
F006 Dietz et al. (1981) selected doses for MEK and sBA based on the earlier
*   pharmacokinetic analysis (Traiger and Bruckner, 1976) that established
*   approximately 96% of an administered dose of sBA was oxidized in vivo to
*   MEK. Thus 1960 mg/kg (2.
F007 Dietz et al. (1981) selected doses for MEK and sBA based on the earlier
*   pharmacokinetic analysis (Traiger and Bruckner, 1976) that established
*   approximately 96% of an administered dose of sBA was oxidized in vivo to
*   MEK. Thus 1960 mg/kg (2.1 ml/kg) of MEK estimates the amount of MEK
*   formed in vivo from a dose of 1776 mg/kg (2.2 ml/kg) of sBA. Male rats
*   were given oral doses of sBA, MEK, 2-3 B-D (or i.v.), or 3H-2B (i.v.) and
*   serial blood samples were collected for up to 30 hours following
*   treatment.
F020 255639
EOR
F002 27
F010 5.0
F004 1
F005 RM
F006 Test Type: Metabolism and Pharmacokinetic Evaluation
**   Strain: Sprague-Dawley
**   Dose Groups/Concentrations: sBA: 2.2 ml/kg or 1776 mg/kg as a 22%
*   aqueous solution (oral). MEK: 2.1ml/kg or 1690 mg/kg as a 21% aqueous
*   solution (oral). 2,3-BD
F007 Test Type: Metabolism and Pharmacokinetic Evaluation
**   Strain: Sprague-Dawley
**   Dose Groups/Concentrations: sBA: 2.2 ml/kg or 1776 mg/kg as a 22%
*   aqueous solution (oral). MEK: 2.1ml/kg or 1690 mg/kg as a 21% aqueous
*   solution (oral). 2,3-BD : 0.68 ml/kg or 676 mg/kg as a 6.8 % aqueous
*   solution (oral or i.v.). 3H-2B: 400 or 800 mg/kg as a 60% aqueous
*   solution (i.v.)
**   Frequency of Treatment: Single Dose (oral or i.v.)
**   Duration of Test: 30 Hours
**   Sex: Male
**   Number/Dose Group: Not Identified
F020 255644
EOR
F002 27
F010 5.0
F004 1
F005 RS
F006 In the sBA-treatment phase of the study, blood concentrations of sBA and
*   its metabolites MEK, 3H-2B, and 2,3-BD were measured. Blood sBA
*   concentrations of 0.59 mg/ml peaked at 2 hours and declined to less than
*   0.05 mg/ml at 16 hours. As th
F007 In the sBA-treatment phase of the study, blood concentrations of sBA and

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*    its metabolites MEK, 3H-2B, and 2,3-BD were measured.  Blood sBA
*    concentrations of 0.59 mg/ml peaked at 2 hours and declined to less than
*    0.05 mg/ml at 16 hours. As the sBA concentration fell, the metabolite
*    concentrations of MEK, 3H-2B, and 2,3-BD concentrations rose to maximums
*    at 8, 12, and 18hr, respectively. The peak concentration of MEK was 0.78
*    mg/ml, while that of 2,3-BD was 0.21 mg/ml. 3H-2B reached a peak
*    concentration of 0.04 mg/ml. Total AUC values for sBA, MEK, 3H-2B, and
*    2,3-BD were 3254 ± 258, 9868 ± 566, 443 ± 93, and 3167 ± 503 mg-hr/l,
*    respectively.
**   Following an oral dose of MEK, blood concentrations of MEK and its
*    metabolites sBA, 3H-2B, and 2,3-BD were measured.  Blood MEK
*    concentrations of 0.95 mg/ml peaked at 4 hours and declined to less than
*    0.07 mg/ml at 18 hours.  As the MEK concentration fell, the end
*    metabolite 2,3-BD rose to a maximum concentration of 0.26 mg/ml at 18
*    hours. Peak concentrations of sBA and 3H-2B were 0.033 and 0.027 mg/ml,
*    respectively. These were detected at 6 and 8 hr after the MEK
*    administration. Total AUC values for MEK, sBA, 3H-2B, and 2,3-BD were
*    10,899 ± 824, 414 ± 38, 382 ± 38, and 3863 ± 238 mg-hr/l, respectively.
F020 255638
EOR
F002 27
F010 5.0
F004 1
F005 TS
F006 2-Butanol (sec-Butanol; sBA) and metabolites 2-Butanone (Methyl ethyl
*    ketone; MEK), 3-Hydroxy-2-Butanone (3H-2B), and 2,3-Butanediol (2,3-BD)
*    (CAS Nos. 78-92-2 (sBA); 78-93-3 (MEK))
**   Purity not identified.
F007 2-Butanol (sec-Butanol; sBA) and metabolites 2-Butanone (Methyl ethyl
*    ketone; MEK), 3-Hydroxy-2-Butanone (3H-2B), and 2,3-Butanediol (2,3-BD)
*    (CAS Nos. 78-92-2 (sBA); 78-93-3 (MEK))
**   Purity not identified.
F020 255643
EOR
F002 27
F010 5.0
F004 2
F005 CL
F006 This study showed the initial metabolism of MEK follows both oxidative
*    and reductive pathways to produce 3-hydroxy-2-butanone, 2,3-butanediol
*    and 2-butanol.
F007 This study showed the initial metabolism of MEK follows both oxidative
*    and reductive pathways to produce 3-hydroxy-2-butanone, 2,3-butanediol
*    and 2-butanol.
F020 255648
EOR
F002 27
F010 5.0
F004 2
F005 RE
F006 DiVincenzo GD, Kaplan CJ and Dedinas J  (1976).  Characterization of the
*    metabolites of Methyl n-Butyl Ketone, Methyl iso-Butyl Ketone, and Methyl
*    Ethyl Ketone in guinea pig serum and their clearance.  Toxicology and
*    Applied Pharmacology 36
F007 DiVincenzo GD, Kaplan CJ and Dedinas J  (1976).  Characterization of the
*    metabolites of Methyl n-Butyl Ketone, Methyl iso-Butyl Ketone, and Methyl
*    Ethyl Ketone in guinea pig serum and their clearance.  Toxicology and
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*    Applied Pharmacology 36, 511-522.
F020 255651
EOR
F002 27
F010 5.0
F004 2
F005 RL
F006 No circumstances occurred that would have affected the quality or
*    integrity of the data.  Test procedures were in accordance with generally
*    accepted scientific standards and described in sufficient detail.
F007 No circumstances occurred that would have affected the quality or
*    integrity of the data.  Test procedures were in accordance with generally
*    accepted scientific standards and described in sufficient detail.
F020 255650
EOR
F002 27
F010 5.0
F004 2
F005 RM
F006 Male guinea pigs ranging in weight from 250 - 450 grams were given a
*    single i.p. dose of 450mg/kg MEK (study also investigated MnBK and MiBK -
*    data not addressed here). Blood was collected by heart puncture from 4
*    animals at each of the fol
F007 Male guinea pigs ranging in weight from 250 - 450 grams were given a
*    single i.p. dose of 450mg/kg MEK (study also investigated MnBK and MiBK -
*    data not addressed here). Blood was collected by heart puncture from 4
*    animals at each of the following times after dose administration: 1, 2,
*    4, 6, 8, 12, and 16 Hr. Only 1 sample was collected from each guinea pig.
*    Serum was separated and refrigerated until assayed within 48 Hr. The
*    concentrations of the ketones and their metabolites were measured in
*    duplicate by direct on-column injection of undiluted serum into a Varian
*    2100 Gas Chromatograph equipped with a flame ionization detector.
*    Ketones and metabolites were quantitated from calibration curves prepared
*    from pure standards.  Greater than 90% of each ketone was distributed in
*    the plasma fraction. Half-lives were estimated by extrapolating the
*    linear portion of the decay curve to zero time.
F020 255647
EOR
F002 27
F010 5.0
F004 2
F005 RM
F006 Test Type:  Metabolism and Pharmacokinetic Evaluation
**   Frequency of Treatment:  Single injection
**   Duration of Test:  16 Hours
**   Number/Dose Group:  4 at each blood - sampling interval
F007 Test Type:  Metabolism and Pharmacokinetic Evaluation
**   Frequency of Treatment:  Single injection
**   Duration of Test:  16 Hours
**   Number/Dose Group:  4 at each blood - sampling interval
F020 255649
EOR
F002 27
F010 5.0
F004 2
F005 RS
F006 MEK: 2-Butanol, 3-hydroxy-2-butanone, and 2,3-butanediol were identified
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*    as metabolites in the serum of guinea pigs injected i.p. with MEK. The
*    half-life of MEK in serum was 270 min. The clearance time of MEK was 12
*    Hr. 2,3-Butanediol was c
F007 MEK: 2-Butanol, 3-hydroxy-2-butanone, and 2,3-butanediol were identified
*    as metabolites in the serum of guinea pigs injected i.p. with MEK. The
*    half-life of MEK in serum was 270 min. The clearance time of MEK was 12
*    Hr. 2,3-Butanediol was cleared in 16 hours, as were the other two
*    metabolites. The metabolism was described as oxidation via hydroxylation
*    of the ? -1 carbon forming 3-hydroxy-2-butanone as the metabolite of MEK.
*    Reduction occurred at the carbonyl group as expected forming the
*    secondary alcohol, 2-butanol from MEK.
F020 255646
EOR
F002 27
F010 5.0
F004 2
F005 TS
F006 2-Butanone (Methyl ethyl ketone; MEK) (CAS No. 78-93-3)
**   Purity:  98% with traces of 2-butanol
F007 2-Butanone (Methyl ethyl ketone; MEK) (CAS No. 78-93-3)
**   Purity:  98% with traces of 2-butanol
F020 255645
EOR
F002 27
F010 5.0
F004 3
F005 CL
F006 Two elimination phases were detected for MEK in blood. The T½ for the
*    faster phase of elimination was 30 min and about 81 min for the slower
*    phase. 2-3% of absorbed dose of MEK was eliminated by exhalation. Urinary
*    excretion of unchanged ME
F007 Two elimination phases were detected for MEK in blood. The T½ for the
*    faster phase of elimination was 30 min and about 81 min for the slower
*    phase. 2-3% of absorbed dose of MEK was eliminated by exhalation. Urinary
*    excretion of unchanged MEK was 0.1% and excretion of the metabolite 2H3B
*    was about 0.1%.
F020 255655
EOR
F002 27
F010 5.0
F004 3
F005 RE
F006 Liira J, Riihimaki V and Pfaffli P  (1988).  Kinetics of methyl ethyl
*    ketone in man: absorption, distribution and elimination in inhalation
*    exposure.  Int.Arch. Occup. Environ. Health 60, 195-200.
F007 Liira J, Riihimaki V and Pfaffli P  (1988).  Kinetics of methyl ethyl
*    ketone in man: absorption, distribution and elimination in inhalation
*    exposure.  Int.Arch. Occup. Environ. Health 60, 195-200.
F020 255658
EOR
F002 27
F010 5.0
F004 3
F005 RL
F006 No circumstances occurred that would have affected the quality or
*    integrity of the data.  Test procedures were in accordance with generally
*    accepted scientific standards and described in sufficient detail.
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F007 No circumstances occurred that would have affected the quality or
*   integrity of the data. Test procedures were in accordance with generally
*   accepted scientific standards and described in sufficient detail.
F020 255657
EOR
F002 27
F010 5.0
F004 3
F005 RM
F006 Nine healthy male volunteers, 18-34 years of age (mean 23.7), weight
*   65-81 kg (mean 74.3), height 172-190 cm (mean 181.8) and calculated
*   surface area 1.81 - 2.09 m2 (mean 1.97) were exposed for 4 Hr to 200ppm
*   MEK on 2 separate days at least
F007 Nine healthy male volunteers, 18-34 years of age (mean 23.7), weight
*   65-81 kg (mean 74.3), height 172-190 cm (mean 181.8) and calculated
*   surface area 1.81 - 2.09 m2 (mean 1.97) were exposed for 4 Hr to 200ppm
*   MEK on 2 separate days at least 1 week apart. Venous blood samples were
*   collected at 1-hr intervals during exposure and over 120 to 210 minutes
*   post-exposure. In a supplementary study, follow-up elimination blood
*   samples were collected in 2 persons until the next morning. One of the
*   exposures constituted sedentary activity and the other encompassed three
*   100 W ergometric exercise periods over minutes 5-15, 95-105 and 225-235
*   during a total exposure of 240 minutes. Exhaled air samples were
*   collected with a 2-way respirator mouthpiece into 4-liter polyester
*   laminated aluminum-foil bags and analyzed immediately. Samples were
*   collected at one-hour intervals during exposure and over 120-210 minutes
*   thereafter. Urine samples were obtained at 2-hour intervals during the
*   exposure day and in separate samples until the next morning. Whole
*   venous blood was analyzed by gas chromatography, as were air samples.
*   Peaks were compared to calibration curves prepared of known blood or air
*   concentrations of MEK. 2-3BD in urine was analyzed according to a
*   modification of the method of Robinson and Reive. The 2 peaks in the
*   chromatograph (d,l-forms and meso-form) were summed for calculations.
F020 255654
EOR
F002 27
F010 5.0
F004 3
F005 RM
F006 Test Type: Metabolism and Pharmacokinetic Evaluation
**   Frequency of Treatment: 2 Exposure periods at least 1 wk between
**   Duration of Test: 4 Hr. Exposure
F007 Test Type: Metabolism and Pharmacokinetic Evaluation
**   Frequency of Treatment: 2 Exposure periods at least 1 wk between
**   Duration of Test: 4 Hr. Exposure
F020 255656
EOR
F002 27
F010 5.0
F004 3
F005 RS
F006 Pulmonary retention of MEK in the lungs remained constant throughout
*   exposure with or without exercise. Relative uptake was 53% ± 2%.
*   Estimated mean total pulmonary uptakes were 11.4 mmol (ventilation volume
*   11 liters/min at rest) and 14.3
F007 Pulmonary retention of MEK in the lungs remained constant throughout
*   exposure with or without exercise. Relative uptake was 53% ± 2%.

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*    Estimated mean total pulmonary uptakes were 11.4 mmol (ventilation volume
*    11 liters/min at rest) and 14.3 mmol (ventilation volume 35 liters/min
*    during the exercise). Blood MEK concentrations increased rapidly during
*    the first hour of exposure (markedly faster when associated with
*    exercise). Thereafter, concentrations increased slowly and linearly
*    through 4 hr with sedentary activity and steeply during the exercise
*    period at the end of the 4 hr exposure period.  Two elimination phases
*    were detected for MEK in blood. The calculated half-time for the faster
*    phase of elimination (0-45 min post-exposure) was 30 min and about 81 min
*    for the slower phase (60-320 min post-exposure). Owing to remarkable
*    solubility of MEK, only 2-3% of absorbed dose was eliminated by
*    exhalation.  Urinary excretion of unchanged MEK was 0.1% and excretion of
*    the metabolite 2H3B was about 0.1%. The authors speculated that the
*    greater part of absorbed MEK is probably converted to products of
*    intermediary metabolism, e.g., to acetate or acetoacetate via 3H2B.
F020 255653
EOR
F002 27
F010 5.0
F004 3
F005 TS
F006 2-Butanone (Methyl ethyl ketone; MEK) (CAS No. 78-93-3)
**   Purity:  Analytical Grade
F007 2-Butanone (Methyl ethyl ketone; MEK) (CAS No. 78-93-3)
**   Purity:  Analytical Grade
F020 255652
EOR
F002 27
F010 5.1.1
F004 1
F005 RE
F006 Environmental Health Criteria 65, World Health Organization,
**    1987.
F007 Environmental Health Criteria 65, World Health Organization,
**    1987.
F008 HEDSET
F009 21-10-1992
F012 20
F020 120141
EOR
F002 27
F010 5.1.1
F004 1
F005 SO
F006 EXXON CHEMICAL, Limited  Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F007 EXXON CHEMICAL, Limited  Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 120142
EOR
F002 27
F010 5.1.1
F004 2
F005 SO
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F006 EXXON CHEMICAL, Limited Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 120143
EOR
F002 27
F010 5.1.1
F004 3
F005 CL
F006 The acute oral LD50 for sBA in Fischer 344 rats is 2193 mg/kg.
F007 The acute oral LD50 for sBA in Fischer 344 rats is 2193 mg/kg.
F008 CLGETTS
F012 20
F020 120144
EOR
F002 27
F010 5.1.1
F004 3
F005 RE
F006 Price, J. B. (1986). Toxicology of industrial chemicals (solvents): The
*   acute oral and percutaneous toxicity, skin and eye irritancy and skin
*   sensitizing potential of secondary butyl alcohol. Shell Research Report
*   SBGR.86.108. Shell Rese
F007 Price, J. B. (1986). Toxicology of industrial chemicals (solvents): The
*   acute oral and percutaneous toxicity, skin and eye irritancy and skin
*   sensitizing potential of secondary butyl alcohol. Shell Research Report
*   SBGR.86.108. Shell Research Limited, Sittingbourne Research Centre.
F008 CLGETTS
F012 20
F020 120145
EOR
F002 27
F010 5.1.1
F004 3
F005 RL
F006 1 - Reliable study without restrictions. No circumstances occurred that
*   would have affected the quality or integrity of the data.
F007 1 - Reliable study without restrictions. No circumstances occurred that
*   would have affected the quality or integrity of the data.
F008 CLGETTS
F012 20
F020 120146
EOR
F002 27
F010 5.1.1
F004 3
F005 RM
F006 Fischer 344 rats were in the age range of 55-65 days when purchased and
*   were 9 -11 weeks old when the study commenced. All animals were fasted
*   for 18 hours prior to dosing and doses were altered by varying the volume
*   dispensed from the syri
F007 Fischer 344 rats were in the age range of 55-65 days when purchased and
*   were 9 -11 weeks old when the study commenced. All animals were fasted

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*    for 18 hours prior to dosing and doses were altered by varying the volume
*    dispensed from the syringe. Body weights were recorded on Days 1, 7 and
*    14. All surviving rats gained weight by the end of the 14-day observation
*    period. The LD50's were calculated using probit analysis
F008 CLGETTS
F012 20
F020 120147
EOR
F002 27
F010 5.1.1
F004 3
F005 RM
F006 Route of Administration:  Oral Gavage
**   Doses:  950 - 2400 mg/kg
**   Volume Administered: Single dose volume varied by body weight
**   Post Dose Observation Period:  Daily for 14 Days
**   Purity:  99.5%
F007 Route of Administration:  Oral Gavage
**   Doses:  950 - 2400 mg/kg
**   Volume Administered: Single dose volume varied by body weight
**   Post Dose Observation Period:  Daily for 14 Days
**   Purity:  99.5%
F008 CLGETTS
F012 20
F020 120148
EOR
F002 27
F010 5.1.1
F004 3
F005 RS
F006 2054 mg/kg (95% fiducial limits, 1283 - 4018 mg/kg) males,
**   2328 mg/kg (95% fiducial limits, 1470 - 5428 mg/kg) females, and
**   2193 mg/kg (95% fiducial limits, 1608 - 4146 mg/kg) combined.
F007 2054 mg/kg (95% fiducial limits, 1283 - 4018 mg/kg) males,
**   2328 mg/kg (95% fiducial limits, 1470 - 5428 mg/kg) females, and
**   2193 mg/kg (95% fiducial limits, 1608 - 4146 mg/kg) combined.
F008 CLGETTS
F012 20
F020 120149
EOR
F002 27
F010 5.1.1
F004 4
F005 CL
F006 The acute oral LD50 for sBA in Carworth-Wistar rats is 6.48 g/kg (5.73 -
*    7.32)
F007 The acute oral LD50 for sBA in Carworth-Wistar rats is 6.48 g/kg (5.73 -
*    7.32)
F008 CLGETTS
F012 20
F020 120150
EOR
F002 27
F010 5.1.1
F004 4
F005 RE
F006 Smyth, H. F. Jr., Carpenter, C. P., Weil, C. S., and Pozzani, U. C.
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*    (1954).  Range-finding toxicity data: List V. Arch Ind Hyg Occup Med,
*    10:61-68.
F007 Smyth, H. F. Jr., Carpenter, C. P., Weil, C. S., and Pozzani, U. C.
*    (1954).  Range-finding toxicity data: List V. Arch Ind Hyg Occup Med,
*    10:61-68.
F008 CLGETTS
F012 20
F020 120151
EOR
F002 27
F010 5.1.1
F004 4
F005 RL
F006 Smyth, H. F. Jr., Carpenter, C. P., Weil, C. S., and Pozzani, U. C.
*    (1954).  Range-finding toxicity data: List V. Arch Ind Hyg Occup Med,
*    10:61-68.
F007 Smyth, H. F. Jr., Carpenter, C. P., Weil, C. S., and Pozzani, U. C.
*    (1954).  Range-finding toxicity data: List V. Arch Ind Hyg Occup Med,
*    10:61-68.
F008 CLGETTS
F012 20
F020 120152
EOR
F002 27
F010 5.1.1
F004 4
F005 RM
F006 Route of Administration:  Oral Gavage
**   Doses:  Logarithmic series
**   Dose Volume Administered:  Single dose; 1-10 ml/rat
**   Post Dose Observation Period:  14 Days
F007 Route of Administration:  Oral Gavage
**   Doses:  Logarithmic series
**   Dose Volume Administered:  Single dose; 1-10 ml/rat
**   Post Dose Observation Period:  14 Days
F008 CLGETTS
F012 20
F020 120153
EOR
F002 27
F010 5.1.1
F004 4
F005 RM
F006 The animals weighed 90 - 120 grams and were not fasted prior to dosing.
*    The most probable LD50 value and the fiducial range were estimated by the
*    method of Thompson using the tables of Weil.
F007 The animals weighed 90 - 120 grams and were not fasted prior to dosing.
*    The most probable LD50 value and the fiducial range were estimated by the
*    method of Thompson using the tables of Weil.
F008 CLGETTS
F012 20
F020 120154
EOR
F002 27
F010 5.1.1
F004 4
F005 RS
```

F006 6.48 g/kg (5.73 - 7.32)
F007 6.48 g/kg (5.73 - 7.32)
F008 CLGETTS
F012 20
F020 120155
EOR
F002 27
F010 5.1.1
F004 5
F005 CL
F006 The reported LD50 was 66 mmol/kg (4890 mg/kg).
F007 The reported LD50 was 66 mmol/kg (4890 mg/kg).
F008 CLGETTS
F012 20
F020 120156
EOR
F002 27
F010 5.1.1
F004 5
F005 RE
F006 Munch, J.C. (1972). Aliphatic alcohols and alkyl esters: narcotic and
*   lethal potencies to tadpoles and to rabbits. Ind. Med. 41:31-33.
F007 Munch, J.C. (1972). Aliphatic alcohols and alkyl esters: narcotic and
*   lethal potencies to tadpoles and to rabbits. Ind. Med. 41:31-33.
F008 CLGETTS
F012 20
F020 120157
EOR
F002 27
F010 5.1.1
F004 5
F005 RE
F006 Munch, J.C. and Schwartze, E.W. (1925). Narcotic and toxic potency of
*   aliphatic alcohols upon rabbits. J Lab Clin Med, 10:985-996.
F007 Munch, J.C. and Schwartze, E.W. (1925). Narcotic and toxic potency of
*   aliphatic alcohols upon rabbits. J Lab Clin Med, 10:985-996.
F008 CLGETTS
F012 20
F020 120158
EOR
F002 27
F010 5.1.1
F004 5
F005 RL
F006 3 - Not Reliable. Study is pre-GLP and documentation insufficient for
*   assessment
F007 3 - Not Reliable. Study is pre-GLP and documentation insufficient for
*   assessment
F008 CLGETTS
F012 20
F020 120159
EOR
F002 27
F010 5.1.1
F004 5
F005 RM
F006 Route of Administration: Oral Gavage

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**   Number of Animals/Dose:  Unknown
**   Doses:  14 or 66 mmol/kg; 1037 or 4890 mg/kg
**   Dose Volume Administered:  < 50 ml
**   Post Dose Observation Period:  24 Hours
F007 Route of Administration:  Oral Gavage
**   Number of Animals/Dose:  Unknown
**   Doses:  14 or 66 mmol/kg; 1037 or 4890 mg/kg
**   Dose Volume Administered:  < 50 ml
**   Post Dose Observation Period:  24 Hours
F008 CLGETTS
F012 20
F020 120160
EOR
F002 27
F010 5.1.1
F004 5
F005 RM
F006 Ten to 35 rabbits weighing between 1.5 and 2.5 kg were given "calculated"
*    quantities of sBA at doses described as the "Narcotic Dose " or "Certain
*    Lethal Dose" by oral gavage and observed for 24 hours.
F007 Ten to 35 rabbits weighing between 1.5 and 2.5 kg were given "calculated"
*    quantities of sBA at doses described as the "Narcotic Dose " or "Certain
*    Lethal Dose" by oral gavage and observed for 24 hours.
F008 CLGETTS
F012 20
F020 120161
EOR
F002 27
F010 5.1.1
F004 5
F005 RM
F006 The cited LD50 [66 mmol/kg, or 4890 mg/kg] is really the Certain Lethal
*    Dose presented in the paper by Munch and Schwartze (1925). The Munch
*    paper (1972) presents the rabbit data reported earlier in 1925 plus
*    tadpole data.  Because of the i
F007 The cited LD50 [66 mmol/kg, or 4890 mg/kg] is really the Certain Lethal
*    Dose presented in the paper by Munch and Schwartze (1925). The Munch
*    paper (1972) presents the rabbit data reported earlier in 1925 plus
*    tadpole data.  Because of the inconsistency in the definition of LD50 and
*    Certain Lethal Dose, a CoR of 3 is assigned to both references.
F008 CLGETTS
F012 20
F020 120162
EOR
F002 27
F010 5.1.1
F004 5
F005 RS
F006 4890 mg/kg
F007 4890 mg/kg
F008 CLGETTS
F012 20
F020 120163
EOR
F002 27
F010 5.1.2
F004 1
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F005 CL
F006 Five of six exposed rats died within 14 days.
F007 Five of six exposed rats died within 14 days.
F008 CLGETTS
F012 20
F020 120164
EOR
F002 27
F010 5.1.2
F004 1
F005 RE
F006 Smyth, H. F. Jr., Carpenter, C. P., Weil, C. S., and Pozzani, U. C.
*   (1954). Range-finding toxicity data: List V. Arch Ind Hyg Occup Med,
*   10:61-68.
F007 Smyth, H. F. Jr., Carpenter, C. P., Weil, C. S., and Pozzani, U. C.
*   (1954). Range-finding toxicity data: List V. Arch Ind Hyg Occup Med,
*   10:61-68.
F008 CLGETTS
F012 20
F020 120165
EOR
F002 27
F010 5.1.2
F004 1
F005 RL
F006 2- Reliable with restrictions. Pre-GLP study documented, meets generally
*   accepted scientific principles, acceptable for assessment.
F007 2- Reliable with restrictions. Pre-GLP study documented, meets generally
*   accepted scientific principles, acceptable for assessment.
F008 CLGETTS
F012 20
F020 120166
EOR
F002 27
F010 5.1.2
F004 1
F005 RM
F006 Route of Administration: Inhalation
**   Observation Period: Up to 14 days
F007 Route of Administration: Inhalation
**   Observation Period: Up to 14 days
F008 CLGETTS
F012 20
F020 120167
EOR
F002 27
F010 5.1.2
F004 1
F005 RM
F006 The study consisted of exposing six male albino rats to a flowing stream
*   of air approaching saturation with sBA vapors. The stream was prepared
*   by proportioning pumps and nominal concentrations (not confirmed by
*   analytical methods) were re
F007 The study consisted of exposing six male albino rats to a flowing stream
*   of air approaching saturation with sBA vapors. The stream was prepared
*   by proportioning pumps and nominal concentrations (not confirmed by
*   analytical methods) were recorded.   The study end point was the

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*    concentration yielding a fractional mortality among six rats within 14
*    days.
F008 CLGETTS
F012 20
F020 120168
EOR
F002 27
F010 5.1.2
F004 1
F005 RS
F006 16,000 ppm sBA was lethal to 5 of 6 rats within 14 days
F007 16,000 ppm sBA was lethal to 5 of 6 rats within 14 days
F008 CLGETTS
F012 20
F020 120169
EOR
F002 27
F010 5.1.2
F004 1
F005 SO
F006 EXXON CHEMICAL, Limited  Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F007 EXXON CHEMICAL, Limited  Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 120170
EOR
F002 27
F010 5.1.2
F004 2
F005 CL
F006 One of six exposed rats died within 14 days.
F007 One of six exposed rats died within 14 days.
F008 CLGETTS
F012 20
F020 120171
EOR
F002 27
F010 5.1.2
F004 2
F005 RE
F006 Mellon (Mellon Institute of Industrial Research). (1951). "Project Report
*    Number 14-78". Union Carbide Corporation, Danbury, CT, USA.
F007 Mellon (Mellon Institute of Industrial Research). (1951). "Project Report
*    Number 14-78". Union Carbide Corporation, Danbury, CT, USA.
F008 CLGETTS
F012 20
F020 120172
EOR
F002 27
F010 5.1.2
F004 2
F005 RL
F006 2- Reliable with restrictions. Pre-GLP study documented, meets generally
*    accepted scientific principles, acceptable for assessment.
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F007 2- Reliable with restrictions. Pre-GLP study documented, meets generally
*   accepted scientific principles, acceptable for assessment.
F008 CLGETTS
F012 20
F020 120173
EOR
F002 27
F010 5.1.2
F004 2
F005 RM
F006 Route of Administration: Inhalation
**   Observation Period: Up to 14 days
F007 Route of Administration: Inhalation
**   Observation Period: Up to 14 days
F008 CLGETTS
F012 20
F020 120174
EOR
F002 27
F010 5.1.2
F004 2
F005 RM
F006 The study consisted of exposing six male albino rats to a flowing stream
*   of air with sBA vapors. The stream was prepared by proportioning pumps
*   and nominal concentrations (not confirmed by analytical methods) were
*   recorded.   The study end
F007 The study consisted of exposing six male albino rats to a flowing stream
*   of air with sBA vapors. The stream was prepared by proportioning pumps
*   and nominal concentrations (not confirmed by analytical methods) were
*   recorded.   The study end point was the concentration yielding a
*   fractional mortality among six rats within 14 days.
F008 CLGETTS
F012 20
F020 120175
EOR
F002 27
F010 5.1.2
F004 2
F005 RS
F006 8,000 ppm sBA was lethal to 1 of 6 rats within 14 days
F007 8,000 ppm sBA was lethal to 1 of 6 rats within 14 days
F008 CLGETTS
F012 20
F020 120176
EOR
F002 27
F010 5.1.2
F004 3
F005 CL
F006 Five of five exposed female rats died following a single 7 hour exposure.
F007 Five of five exposed female rats died following a single 7 hour exposure.
F008 CLGETTS
F012 20
F020 120177
EOR
F002 27
F010 5.1.2

F004 3
F005 RE
F006 Nelson, B. K., Brightwell, W. S., Khan, A., Burg, J. R., and Goad, P. T.
* (1989). Lack of selective developmental toxicity of three butanol
* isomers administered by inhalation to rats. Fundam Appl Toxicol,
* 12:469-479.
F007 Nelson, B. K., Brightwell, W. S., Khan, A., Burg, J. R., and Goad, P. T.
* (1989). Lack of selective developmental toxicity of three butanol
* isomers administered by inhalation to rats. Fundam Appl Toxicol,
* 12:469-479.
F008 CLGETTS
F012 20
F020 120178
EOR
F002 27
F010 5.1.2
F004 3
F005 RL
F006 2 - Reliable. Pilot study with acceptable restrictions.
F007 2 - Reliable. Pilot study with acceptable restrictions.
F008 CLGETTS
F012 20
F020 120179
EOR
F002 27
F010 5.1.2
F004 3
F005 RM
F006 Study Type: Acute Inhalation (Pilot for Teratology study)
** Purity: >or= 99 %
** Route of Administration: Inhalation
** Observation Period: Unknown
F007 Study Type: Acute Inhalation (Pilot for Teratology study)
** Purity: >or= 99 %
** Route of Administration: Inhalation
** Observation Period: Unknown
F008 CLGETTS
F012 20
F020 120180
EOR
F002 27
F010 5.1.2
F004 3
F005 RM
F006 The study consisted of exposing five female rats to a flowing stream of
* air with sBA vapors. The stream was prepared by proportioning pumps. The
* study end point was the concentration yielding a fractional mortality.
F007 The study consisted of exposing five female rats to a flowing stream of
* air with sBA vapors. The stream was prepared by proportioning pumps. The
* study end point was the concentration yielding a fractional mortality.
F008 CLGETTS
F012 20
F020 120181
EOR
F002 27
F010 5.1.2
F004 3

F005 RS
F006 10,000 ppm sBA was lethal to 5 of 5 rats
F007 10,000 ppm sBA was lethal to 5 of 5 rats
F008 CLGETTS
F012 20
F020 120182
EOR
F002 27
F010 5.1.2
F004 4
F005 CL
F006 Doses from 3,300 to 19,800 ppm induced narcosis but not death.
F007 Doses from 3,300 to 19,800 ppm induced narcosis but not death.
F008 CLGETTS
F012 20
F020 120183
EOR
F002 27
F010 5.1.2
F004 4
F005 RE
F006 Starrek, E. (1938). Dissertation, Wirzburg.
F007 Starrek, E. (1938). Dissertation, Wirzburg.
F008 CLGETTS
F012 20
F020 120184
EOR
F002 27
F010 5.1.2
F004 4
F005 RL
F006 4 - Documentation insufficient for assessment. Non-guideline pre-GLP
*   study.
F007 4 - Documentation insufficient for assessment. Non-guideline pre-GLP
*   study.
F008 CLGETTS
F012 20
F020 120185
EOR
F002 27
F010 5.1.2
F004 4
F005 RM
F006 1650 ppm: no signs of intoxication after 420 minutes.
**   3300 ppm: ataxia in 51-100 minutes, prostration in 120-180 minutes,
*   narcosis in 3000 minutes, no deaths
**   19,800 ppm: ataxia in 7-8 minutes, prostration in 12-20 minutes, narcosis
*   in 40 m
F007 1650 ppm: no signs of intoxication after 420 minutes.
**   3300 ppm: ataxia in 51-100 minutes, prostration in 120-180 minutes,
*   narcosis in 3000 minutes, no deaths
**   19,800 ppm: ataxia in 7-8 minutes, prostration in 12-20 minutes, narcosis
*   in 40 minutes, no deaths
F008 CLGETTS
F012 20
F020 120186
EOR

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F002 27
F010 5.1.2
F004 4
F005 RM
F006 Route of Administration:  Inhalation
**   Doses/time: 1650, 3300, 19800 ppm/decreasing lengths of time
**   Post Dose Observation Period:  Various
F007 Route of Administration:  Inhalation
**   Doses/time: 1650, 3300, 19800 ppm/decreasing lengths of time
**   Post Dose Observation Period:  Various
F008 CLGETTS
F012 20
F020 120187
EOR
F002 27
F010 5.1.2
F004 4
F005 RS
F006 Not Defined
F007 Not Defined
F008 CLGETTS
F012 20
F020 120188
EOR
F002 27
F010 5.1.3
F004 1
F005 CL
F006 The acute percutaneous LD50 of undiluted sBA in rats was > 2000 mg/kg.
F007 The acute percutaneous LD50 of undiluted sBA in rats was > 2000 mg/kg.
F008 CLGETTS
F012 20
F020 120189
EOR
F002 27
F010 5.1.3
F004 1
F005 RE
F006 Price, J. B. (1986).  Toxicology of industrial chemicals (solvents): The
*    acute oral and percutaneous toxicity, skin and eye irritancy and skin
*    sensitizing potential of secondary butyl alcohol.  Shell research Report
*    SBGR.86.108.  Shell Rese
F007 Price, J. B. (1986).  Toxicology of industrial chemicals (solvents): The
*    acute oral and percutaneous toxicity, skin and eye irritancy and skin
*    sensitizing potential of secondary butyl alcohol.  Shell research Report
*    SBGR.86.108.  Shell Research Limited, Sittingbourne Research Centre.
F008 CLGETTS
F012 20
F020 120190
EOR
F002 27
F010 5.1.3
F004 1
F005 RL
F006 1 - Reliable without Restrictions.  No circumstances occurred that would
*    have affected the quality or integrity of the data.
F007 1 - Reliable without Restrictions.  No circumstances occurred that would
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*    have affected the quality or integrity of the data.
F008 CLGETTS
F012 20
F020 120191
EOR
F002 27
F010 5.1.3
F004 1
F005 RM
F006 Fischer 344 rats were in the age range of 55-65 days when purchased and
*    were 9 -11 weeks old when the study commenced.  The day before dosing the
*    animals, approximately 60% of the dorsal hair was closely shorn with fine
*    electric clippers, a
F007 Fischer 344 rats were in the age range of 55-65 days when purchased and
*    were 9 -11 weeks old when the study commenced.  The day before dosing the
*    animals, approximately 60% of the dorsal hair was closely shorn with fine
*    electric clippers, and the rats and the rats were weighed on the day of
*    dosing.  Varying the volume dispensed from the syringe altered doses.
*    Application was made at room temperature and the test material was
*    covered with aluminum foil and held in place by a double over-wrap of
*    waterproof adhesive tape. The rats were individually housed for the next
*    24 hours.  Food was withheld, but water was available ad libitum.  At the
*    end of the 24-hour period, the tape and foil were removed and the skin
*    was washed with warm dilute detergent solution and then dried.  The
*    animals were observed for signs of toxicity for 14 days after dosing.
*    Body weights were recorded on Days 1, 7 and 14.  None of the rats died.
*    There were no overt signs of toxicity and all rats gained weight relative
*    to their day 1body weight.
F008 CLGETTS
F012 20
F020 120192
EOR
F002 27
F010 5.1.3
F004 1
F005 RM
F006 Route of Administration:  Dermal
**   Doses/time:  2000 mg/kg single application / 24-hour occlusive patch
**   Post Dose Observation Period:  Daily for 14 Days
**   Purity:  99.5%
F007 Route of Administration:  Dermal
**   Doses/time:  2000 mg/kg single application / 24-hour occlusive patch
**   Post Dose Observation Period:  Daily for 14 Days
**   Purity:  99.5%
F008 CLGETTS
F012 20
F020 120193
EOR
F002 27
F010 5.1.3
F004 1
F005 RS
F006 > 2000 mg/kg
F007 > 2000 mg/kg
F008 CLGETTS
F012 20
F020 120194
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EOR
F002 27
F010 5.1.4
F004 1
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 120195
EOR
F002 27
F010 5.10
F004 1
F005 RE
F006 Environmental Health Criteria 65. Butanols: Four Isomers.
**   World Health Organization, 1987.
F007 Environmental Health Criteria 65. Butanols: Four Isomers.
**   World Health Organization, 1987.
F008 HEDSET
F009 22-10-1992
F012 20
F020 120203
EOR
F002 27
F010 5.10
F004 1
F005 RM
F006 Excessive exposure by inhalation may result in headache,
**   dizziness, drowsiness and narcosis. No adverse systemic
**   effects due to exposure to 2-butanol have been reported in
**   man.
F007 Excessive exposure by inhalation may result in headache,
**   dizziness, drowsiness and narcosis. No adverse systemic
**   effects due to exposure to 2-butanol have been reported in
**   man.
F008 HEDSET
F009 22-10-1992
F012 20
F020 120204
EOR
F002 27
F010 5.10
F004 1
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 120205
EOR

F002 27
F010 5.11
F004 1
F005 CL
F006 sBA caused a concentration-dependent decrease in respiratory tidal volume
* in normal and cannulated mice and acts as a respiratory irritant.
F007 sBA caused a concentration-dependent decrease in respiratory tidal volume
* in normal and cannulated mice and acts as a respiratory irritant.
F008 CLGETTS
F012 20
F020 120196
EOR
F002 27
F010 5.11
F004 1
F005 RE
F006 Hansen, L.F., and Nielsen, G.D. (1994). Sensory irritation, pulmonary
* irritation and structure-activity relationships of alcohols. Toxicol.,
* 88:81-99.
F007 Hansen, L.F., and Nielsen, G.D. (1994). Sensory irritation, pulmonary
* irritation and structure-activity relationships of alcohols. Toxicol.,
* 88:81-99.
F008 CLGETTS
F012 20
F020 120197
EOR
F002 27
F010 5.11
F004 1
F005 RL
F006 1 - Reliable without Restrictions. No circumstances occurred that would
* have affected the quality or integrity of the data.
F007 1 - Reliable without Restrictions. No circumstances occurred that would
* have affected the quality or integrity of the data.
F008 CLGETTS
F012 20
F020 120198
EOR
F002 27
F010 5.11
F004 1
F005 RM
F006 Respiratory rates of CF-1 mice (mean weight 25 g.) were determined prior
* to exposure. SBA was evaporated, diluted with room air and fed into a 3.3
* liter chamber at an airflow rate of 18.3 to 26.9 l/min. Each animal was
* placed in a body ple
F007 Respiratory rates of CF-1 mice (mean weight 25 g.) were determined prior
* to exposure. SBA was evaporated, diluted with room air and fed into a 3.3
* liter chamber at an airflow rate of 18.3 to 26.9 l/min. Each animal was
* placed in a body plethysmograph attached to the exposure chamber so that
* the head of the animal protruded into the chamber. The respiratory rate
* and the relative tidal volume were obtained by attaching a pressure
* transducer to each plethysmograph. The results were expressed as
* percentage of pre-exposure values, obtained from a 10-minute control
* period. The exposure was 30 minutes, followed by a 20-minute recovery
* period during which the respiratory pattern and respiratory rate were
* monitored continuously. Respiration rates and tidal volumes were compared

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*    between normal and cannulated mice to determine the on-set and extent of
*    respiratory irritation. In the cannulated mice, the onset of the decrease
*    in respiration was slower than that of the normal mice indicating that
*    sBA was acting as a respiratory irritant.
F008 CLGETTS
F012 20
F020 120199
EOR
F002 27
F010 5.11
F004 1
F005 RM
F006 Species/Strain:  Mouse / CF-1
**   Sex:  Male
**   Number/Sex/Dose:  10
**   Vehicle:  None
**   Route of Administration:  Inhalation
**   Doses:  2800, 5600, 10100 or 15300 ppm normal mice;
**   10500 or 14000 ppm cannulated mice
**   Time of Exposure:  30 minute
**   Post Dose
F007 Species/Strain:  Mouse / CF-1
**   Sex:  Male
**   Number/Sex/Dose:  10
**   Vehicle:  None
**   Route of Administration:  Inhalation
**   Doses:  2800, 5600, 10100 or 15300 ppm normal mice;
**   10500 or 14000 ppm cannulated mice
**   Time of Exposure:  30 minute
**   Post Dose Observation Period:  20 minute
**   Method:  Alarie Test
**   GLP:  Unknown
**   Year:  1994
F008 CLGETTS
F012 20
F020 120200
EOR
F002 27
F010 5.11
F004 1
F005 RS
F006 640 ppm RD0 Threshold Concentration at 2 minutes;
**   11800 ppm RD50 at 10 minutes
F007 640 ppm RD0 Threshold Concentration at 2 minutes;
**   11800 ppm RD50 at 10 minutes
F008 CLGETTS
F012 20
F020 120201
EOR
F002 27
F010 5.11
F004 1
F005 TS
F006 sec-Butanol (sBA)
F007 sec-Butanol (sBA)
F008 CLGETTS
F012 20
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F020 120202
EOR
F002 27
F010 5.2.1
F004 1
F005 RE
F006 Environmental Health Criteria 65, Butanols: Four Isomers.
** World Health Organization, 1987.
F007 Environmental Health Criteria 65, Butanols: Four Isomers.
** World Health Organization, 1987.
F008 HEDSET
F009 21-10-1992
F012 20
F020 120206
EOR
F002 27
F010 5.2.1
F004 1
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
** EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
** EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 120207
EOR
F002 27
F010 5.2.1
F004 2
F005 CL
F006 sBA caused no skin reaction and is not a skin irritant in rabbits.
F007 sBA caused no skin reaction and is not a skin irritant in rabbits.
F008 CLGETTS
F012 20
F020 120208
EOR
F002 27
F010 5.2.1
F004 2
F005 RE
F006 Price, J. B. (1986). Toxicology of industrial chemicals (solvents): The
* acute oral and percutaneous toxicity, skin and eye irritancy and skin
* sensitizing potential of secondary butyl alcohol. Shell research Report
* SBGR.86.108. Shell Rese
F007 Price, J. B. (1986). Toxicology of industrial chemicals (solvents): The
* acute oral and percutaneous toxicity, skin and eye irritancy and skin
* sensitizing potential of secondary butyl alcohol. Shell research Report
* SBGR.86.108. Shell Research Limited, Sittingbourne Research Centre.
F008 CLGETTS
F012 20
F020 120209
EOR
F002 27
F010 5.2.1
F004 2

F005 RL
F006 1 - Reliable without Restrictions. No circumstances occurred that would
*   have affected the quality or integrity of the data
F007 1 - Reliable without Restrictions. No circumstances occurred that would
*   have affected the quality or integrity of the data
F008 CLGETTS
F012 20
F020 120210
EOR
F002 27
F010 5.2.1
F004 2
F005 RM
F006 New Zealand White rabbits, 3 - 6 months of age, were acclimated to the
*   laboratory conditions for at least 2 weeks prior to experiment
*   initiation. The hair of the dorsal back between the shoulders and
*   hindquarters of three male and 3 female
F007 New Zealand White rabbits, 3 - 6 months of age, were acclimated to the
*   laboratory conditions for at least 2 weeks prior to experiment
*   initiation. The hair of the dorsal back between the shoulders and
*   hindquarters of three male and 3 female rabbits, 4 - 9 months of age at
*   dosing, was closely shorn with fine electric clippers. A test site was
*   selected and a 2 cm x 2 cm lint patch with 0.5 ml of sBA was applied to
*   it. The patch and surrounding skin were covered by a single layer of
*   gauze and held in place with an elastic adhesive bandage. The wrapping
*   and patch were removed after 4 hours and the skin was not washed. The
*   site was examined and scored for erythema and edema on a graded scale 0 -
*   4. Observations were made 30 minutes after the removal of the patch and
*   at 24, 48, and 72 hours and 7 days following dosing. The mean scores for
*   each rabbit at each observation time were calculated. There were no skin
*   reactions following the application of sBA to rabbit skin for 4 hours.
*   The test material is therefore not a skin irritant in rabbits.
F008 CLGETTS
F012 20
F020 120211
EOR
F002 27
F010 5.2.1
F004 2
F005 RM
F006 Purity: 99.5%
**   Sex: Male and Female
**   Vehicle: None
**   Route of Administration: Dermal
**   Doses: 0.5 ml
**   Doses/Time: Single application
**   Post Dose Observation Period: After removal of patch: 0.5 hours; 24, 48,
*   72 hours and Day 7 after dosing.
F007 Purity: 99.5%
**   Sex: Male and Female
**   Vehicle: None
**   Route of Administration: Dermal
**   Doses: 0.5 ml
**   Doses/Time: Single application
**   Post Dose Observation Period: After removal of patch: 0.5 hours; 24, 48,
*   72 hours and Day 7 after dosing.
F008 CLGETTS

F012 20
F020 120212
EOR
F002 27
F010 5.2.1
F004 2
F005 RS
F006 PII = 0
F007 PII = 0
F008 CLGETTS
F012 20
F020 120213
EOR
F002 27
F010 5.2.2
F004 1
F005 CL
F006 sBA caused moderate damage and/or corneal opacity in rabbits.
F007 sBA caused moderate damage and/or corneal opacity in rabbits.
F008 CLGETTS
F012 20
F020 120214
EOR
F002 27
F010 5.2.2
F004 1
F005 RE
F006 Carpenter, C.P., and Smith, H. F. Jr,. (1946). Chemical Burns of the
* Rabbit Cornea. Am. J. Ophth. 29:1363.
F007 Carpenter, C.P., and Smith, H. F. Jr,. (1946). Chemical Burns of the
* Rabbit Cornea. Am. J. Ophth. 29:1363.
F008 CLGETTS
F012 20
F020 120215
EOR
F002 27
F010 5.2.2
F004 1
F005 RE
F006 Smyth, H. F. Jr, Carpenter, C. P., Weil, C. S., and Pozzani, U. C.
* (1954). Range-finding toxicity data: List V. Arch Ind Hyg Occup Med,
* 10:61-68.
F007 Smyth, H. F. Jr, Carpenter, C. P., Weil, C. S., and Pozzani, U. C.
* (1954). Range-finding toxicity data: List V. Arch Ind Hyg Occup Med,
* 10:61-68.
F008 CLGETTS
F012 20
F020 120216
EOR
F002 27
F010 5.2.2
F004 1
F005 RL
F006 2 - Reliable with restrictions: data are from a collection of data.
F007 2 - Reliable with restrictions: data are from a collection of data.
F008 CLGETTS
F012 20

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F020 120217
EOR
F002 27
F010 5.2.2
F004 1
F005 RM
F006 Eye injury in rabbits records the degree of corneal narcosis from various
*    volumes and concentrations of chemical, as detailed in Carpenter and
*    Smyth (1946).  Grade 1 indicates at most a very small area of narcosis
*    resulting from 0.5 ml of u
F007 Eye injury in rabbits records the degree of corneal narcosis from various
*    volumes and concentrations of chemical, as detailed in Carpenter and
*    Smyth (1946).  Grade 1 indicates at most a very small area of narcosis
*    resulting from 0.5 ml of undiluted chemical in the eye; Grade 5 indicates
*    a so-called severe burn from 0.005 ml, and Grade 10 indicates a severe
*    burn from 0.5 ml of a 1% solution in water or propylene glycol.
F008 CLGETTS
F012 20
F020 120218
EOR
F002 27
F010 5.2.2
F004 1
F005 RM
F006 Sex:  Male
**   Vehicle:  None
**   Route of Administration:  Ocular application into the conjunctival sac of
*    one eye
**   Control:  Untreated eye
**   Dose:  Single application of undiluted sBA
**   Volume:  0.02 and 0.1 ml
**   Post Dose Observation Period:  24 Hours
F007 Sex:  Male
**   Vehicle:  None
**   Route of Administration:  Ocular application into the conjunctival sac of
*    one eye
**   Control:  Untreated eye
**   Dose:  Single application of undiluted sBA
**   Volume:  0.02 and 0.1 ml
**   Post Dose Observation Period:  24 Hours
F008 CLGETTS
F012 20
F020 120219
EOR
F002 27
F010 5.2.2
F004 1
F005 RS
F006 Irritating (score 4/10); Severe injury from 0.1 ml, minor from 0.02 ml;
*    Grade 4 eye injury.
F007 Irritating (score 4/10); Severe injury from 0.1 ml, minor from 0.02 ml;
*    Grade 4 eye injury.
F008 CLGETTS
F012 20
F020 120220
EOR
F002 27
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F010 5.2.2
F004 1
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
** EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
** EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 120221
EOR
F002 27
F010 5.2.2
F004 2
F005 CL
F006 sBA caused moderate conjunctival inflammation in all six rabbits with
* slight transitory iritic damage and/or corneal opacity in three rabbits.
* One rabbit developed intense, extensive corneal opacity and complete loss
* of iritic response. T
F007 sBA caused moderate conjunctival inflammation in all six rabbits with
* slight transitory iritic damage and/or corneal opacity in three rabbits.
* One rabbit developed intense, extensive corneal opacity and complete loss
* of iritic response. The test material was there for corrosive to the
* rabbit eye. On administration of sBA, there was a moderate initial pain
* response.
F008 CLGETTS
F012 20
F020 120222
EOR
F002 27
F010 5.2.2
F004 2
F005 RE
F006 Price, J. B. (1986). Toxicology of industrial chemicals (solvents): The
* acute oral and percutaneous toxicity, skin and eye irritancy and skin
* sensitizing potential of secondary butyl alcohol. Shell research Report
* SBGR.86.108. Shell Rese
F007 Price, J. B. (1986). Toxicology of industrial chemicals (solvents): The
* acute oral and percutaneous toxicity, skin and eye irritancy and skin
* sensitizing potential of secondary butyl alcohol. Shell research Report
* SBGR.86.108. Shell Research Limited, Sittingbourne Research Centre.
F008 CLGETTS
F012 20
F020 120223
EOR
F002 27
F010 5.2.2
F004 2
F005 RL
F006 1 - Reliable without Restrictions. No circumstances occurred that would
* have affected the quality or integrity of the data.
F007 1 - Reliable without Restrictions. No circumstances occurred that would
* have affected the quality or integrity of the data.
F008 CLGETTS
F012 20
F020 120224

EOR
F002 27
F010 5.2.2
F004 2
F005 RM
F006 New Zealand White rabbits, 3 - 6 months of age, were acclimated to the
*   laboratory conditions for at least 2 weeks prior to experiment
*   initiation. Three male and 3 female rabbits were 4 - 9 months of age at
*   dosing. The day before testing, t
F007 New Zealand White rabbits, 3 - 6 months of age, were acclimated to the
*   laboratory conditions for at least 2 weeks prior to experiment
*   initiation. Three male and 3 female rabbits were 4 - 9 months of age at
*   dosing. The day before testing, the eyes were carefully examined for any
*   damage and any animals showing damage were replaced. A single dose of
*   0.1 ml of sBA was placed into the lower conjunctival sac of one eye and
*   the lids held together for a few seconds to prevent loss of material.
*   The eyes were not washed. The reactions of the animal were observed and
*   the initial pain responses graded on a 1 - 6 scale, no pain to very sever
*   initial pain. Visual assessments were made 1, 5-7, 24, 28, and 72 hours
*   and 7 Days postdosing. Irritancy was scored for the cornea, iris, and
*   conjunctiva using standard scores. Any corneal damage visualization was
*   aided by instillation of one drop of 2% fluorescein solution. The degree
*   of irritation was classified using a scheme based on the OECD Data
*   Interpretation Guide (1984). The instillation of undiluted sBA resulted
*   in moderate initial pain. The conjunctival redness, chemosis and
*   discharge, corneal opacity and damage to the iris were assessed and mean
*   scores calculated. All rabbits had moderate conjunctival inflammation
*   with some discharge within 1 hour of dosing. The swelling and discharge
*   largely cleared by four hours but the redness persisted in 3 rabbits for
*   7 days. These 3 animals, and another, had impaired iritic response
*   and/or slight corneal opacity between 24 and 72 hours postdosing. The
*   effect had cleared by 7 days in 3 rabbits. The severely affected rabbit
*   had a completely opaque cornea and no iritic response. It was humanely
*   terminated since recovery was deemed not possible. The remaining rabbits
*   were retained and by day 14 all ocular effects had cleared. In view of
*   the responses, sBA is classified as corrosive to rabbit eyes (OECD, 1984).
F008 CLGETTS
F012 20
F020 120225
EOR
F002 27
F010 5.2.2
F004 2
F005 RM
F006 Study Type: Ocular Irritation (Draize type)
**   Purity: 99.5%
**   Sex: Male and Female
**   Vehicle: None
**   Route of Administration: Ocular application into the conjunctival sac of
*   one eye
**   Control: Untreated Eye
**   Dose: Single application of neat ma
F007 Study Type: Ocular Irritation (Draize type)
**   Purity: 99.5%
**   Sex: Male and Female
**   Vehicle: None
**   Route of Administration: Ocular application into the conjunctival sac of

```
*    one eye
**   Control:  Untreated Eye
**   Dose:  Single application of neat material
**   Volume:  0.1 ml
**   Post Dose Observation Period:  1, 5-7, 24, 28, and 72 hours and 7 Days
*    postdosing
F008 CLGETTS
F012 20
F020 120226
EOR
F002 27
F010 5.2.2
F004 2
F005 RS
F006 Corrosive
F007 Corrosive
F008 CLGETTS
F012 20
F020 120227
EOR
F002 27
F010 5.3
F004 1
F005 CL
F006 In the guinea pig maximization test of Magnusson and Kligman, sBA did not
*    induce positive responses in any of the 20 test animals at 24 or 48 hours
*    after removal of the challenge patches.  sBA is therefore not a dermal
*    sensitizer in guinea
F007 In the guinea pig maximization test of Magnusson and Kligman, sBA did not
*    induce positive responses in any of the 20 test animals at 24 or 48 hours
*    after removal of the challenge patches.  sBA is therefore not a dermal
*    sensitizer in guinea pigs.
F008 CLGETTS
F012 20
F020 120228
EOR
F002 27
F010 5.3
F004 1
F005 RE
F006 Price, J. B. (1986).  Toxicology of industrial chemicals (solvents): The
*    acute oral and percutaneous toxicity, skin and eye irritancy and skin
*    sensitizing potential of secondary butyl alcohol.  Shell research Report
*    SBGR.86.108.  Shell Rese
F007 Price, J. B. (1986).  Toxicology of industrial chemicals (solvents): The
*    acute oral and percutaneous toxicity, skin and eye irritancy and skin
*    sensitizing potential of secondary butyl alcohol.  Shell research Report
*    SBGR.86.108.  Shell Research Limited, Sittingbourne Research Centre.
F008 CLGETTS
F012 20
F020 120229
EOR
F002 27
F010 5.3
F004 1
F005 RL
F006 1 - Reliable without Restrictions.  No circumstances occurred that would
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*    have affected the quality or integrity of the data.
F007 1 - Reliable without Restrictions.  No circumstances occurred that would
*    have affected the quality or integrity of the data.
F008 CLGETTS
F012 20
F020 120230
EOR
F002 27
F010 5.3
F004 1
F005 RM
F006 Guinea pigs in the weight range of 300-370 grams were purchased from a
*    commercial supplier and acclimated to the laboratory for at least 2
*    weeks.  The skin sensitization potential of sBA was assessed using the
*    guinea pig maximization test o
F007 Guinea pigs in the weight range of 300-370 grams were purchased from a
*    commercial supplier and acclimated to the laboratory for at least 2
*    weeks.  The skin sensitization potential of sBA was assessed using the
*    guinea pig maximization test of Magnusson and Kligman.  The test was
*    accomplished in 2 stages: rangefinding and definitive test.
**
**   Rangefinding:
**   The purpose of the rangefinding studies was to determine the
*    concentrations of test material to be used for intradermal induction,
*    topical induction and topical challenge.  Two males and two female guinea
*    pigs were closely shorn in the shoulder region using electric clippers
*    followed by an electric razor and 0.1 ml of several dilutions (0.05, 0.1,
*    0.5 and 1.0% [m/v] in corn oil) of sBA injected intradermally each side
*    of the midline.  The animals were observed over the next few days to
*    determine the maximum concentration that could be tolerated without
*    causing untoward toxicity.  Three further groups of two males and two
*    females had their flanks closely shorn and 0.3 ml of several dilutions
*    (25%, 50%, and 75% [m/v] in corn oil) of sBA were applied to a 4 cm x 4
*    cm Whatman Number 3 filter paper patches.  The patches were placed on the
*    flanks and held in place with a "Sleek" adhesive tape patch, then covered
*    with a "Poroplast" elastic adhesive bandage for 24 hours.  The bandages
*    were removed and the animals were examined for signs of irritation and
*    scored using a 4-point scale (0, 1, 2, and 3).  The concentration used
*    for topical induction was the one that scored 1 for irritation and the
*    concentration for challenge was the one that was 0, a non-irritant.
**
**   Definitive:
**   This test was conducted using a group of ten male and ten female guinea
*    pigs together with a control group of five males and five females.  The
*    test consisted of two stages: a) induction by intradermal injection and
*    topical application, and, 2) topical challenge.  The following
*    concentrations were selected for the definitive study: Intradermal
*    induction, 0.1% (m/v) in corn oil; Topical induction (one week following
*    intradermal challenge), 50% (m/v) in corn oil and 25% (m/v) in corn oil.
*    Topical challenge was carried out two weeks following the topical
*    induction by applying 0.1 ml of the diluted sBA to a semi-occluded
*    challenge patch and removing it 24 hours later. The erythema resulting
*    from the topical challenge was scored on a 4-point scale (0, 1, 2, and 3)
*    immediately on removal of the challenge patches and 24 and 48 hours
*    latter.  None of the twenty test animals showed any positive response at
*    either 24 or 48 hours after the removal of the challenge patches.  It was
*    concluded that sBA was not a dermal sensitizer in guinea pigs.
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F008 CLGETTS
F012 20
F020 120231
EOR
F002 27
F010 5.3
F004 1
F005 RM
F006 Purity: 99.5%
**
**   Sex: Male and Female
**
**   Route of Administration: Intradermal and topical induction; topical
*   challenge
**
**   Doses:
**   Intradermal Induction:
**   Test Doses:
**   2 injections (0.1 ml) of Freund's Complete Adjuvant (FCA)
**   2 injections (0.1 ml
F007 Purity: 99.5%
**
**   Sex: Male and Female
**
**   Route of Administration: Intradermal and topical induction; topical
*   challenge
**
**   Doses:
**   Intradermal Induction:
**   Test Doses:
**   2 injections (0.1 ml) of Freund's Complete Adjuvant (FCA)
**   2 injections (0.1 ml) of sBA in corn oil
**   2 injections (0.1 ml) of sBA in 50:50 FCA:corn oil
**   Control Doses:
**   2 injections (0.1 ml) of Freund's Complete Adjuvant (FCA)
*   2 injections (0.1
*   ml) of corn oil
**   2 injections (0.1 ml) of 50:50 FCA:corn oil
**   Topical Induction:
**   Application of 0.3 ml 50% sBA (m/v) in corn oil and, 25% sBA (m/v) in
*   corn oil covered for 48 hours.
**   Topical Challenge:
**   Application 0.1 ml of diluted sBA to a semi-occluded challenge patch and
*   removing it 24 hours later.
**
**   Post Dose Observation Period: Immediately, 24 and 48 hours following
*   challenge
F008 CLGETTS
F012 20
F020 120232
EOR
F002 27
F010 5.3
F004 1
F005 RS
F006 sBA is not a dermal sensitizer in guinea pigs.
F007 sBA is not a dermal sensitizer in guinea pigs.

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F008 CLGETTS
F012 20
F020 120233
EOR
F002 27
F010 5.3
F004 2
F005 CL
F006 In the guinea pig maximization test of Magnusson and Kligman, sBA is not
*    a dermal sensitizer.
F007 In the guinea pig maximization test of Magnusson and Kligman, sBA is not
*    a dermal sensitizer.
F008 CLGETTS
F012 20
F020 120234
EOR
F002 27
F010 5.3
F004 2
F005 RE
F006 Elf Atochem, Centre International de Toxicologie.  1997.  Skin
*    sensitization in guinea pigs (Maximization method of Magnusson, B. and
*    Kligman, A.M.).  Report # 14861 TSG.
F007 Elf Atochem, Centre International de Toxicologie.  1997.  Skin
*    sensitization in guinea pigs (Maximization method of Magnusson, B. and
*    Kligman, A.M.).  Report # 14861 TSG.
F008 CLGETTS
F012 20
F020 120235
EOR
F002 27
F010 5.3
F004 2
F005 RL
F006 1 - Reliable without Restrictions.
F007 1 - Reliable without Restrictions.
F008 CLGETTS
F012 20
F020 120236
EOR
F002 27
F010 5.3
F004 2
F005 RM
F006 Age:  ~ 3 months
**
**   Sex:  Male and Female
**
**   Weight (initial):  Males 335 ± 17 g; Females 332 ± 19 g
**
**   Doses:
**   Intradermal Induction:
**   Test Doses:
**   Injections: sBA in paraffin oil (5% w/w)
**   sBA in FCA (Freund's Complete Adjuvant)
**   Control Doses:
**   In
```

F007 Age: ~ 3 months
**
**   Sex: Male and Female
**
**   Weight (initial): Males 335 ± 17 g; Females 332 ± 19 g
**
**   Doses:
**   Intradermal Induction:
**   Test Doses:
**   Injections: sBA in paraffin oil (5% w/w)
**   sBA in FCA (Freund's Complete Adjuvant)
**   Control Doses:
**   Injections: Paraffin oil
**   Freund's Complete Adjuvant (FCA)
**   Topical Induction:
**   Application: sBA (undiluted) covered for 48 hours
**   Topical Challenge:
**   Application: sBA (undiluted) covered for 24 hours
**
**   Post Dose Observation Period: Skin reactions were evaluated at
*   approximately 24 and 48 hours.
F008 CLGETTS
F012 20
F020 120237
EOR
F002 27
F010 5.3
F004 2
F005 RM
F006 Clinical Signs: None
**
**   Rechallenge: None
**
**   Thirty guinea pigs were allocated to two groups: a control group 1 (five
*   males and five females) and a treated group 2 (ten males and ten
*   females).
**   Day 1: Intradermal injections of Freund's complete
F007 Clinical Signs: None
**
**   Rechallenge: None
**
**   Thirty guinea pigs were allocated to two groups: a control group 1 (five
*   males and five females) and a treated group 2 (ten males and ten
*   females).
**   Day 1: Intradermal injections of Freund's complete adjuvant mixed with
*   the test substance (treated group) or the vehicle (control group) were
*   performed in the dorsal region between the shoulders. Day 7: The same
*   dorsal region between the shoulders received a topical application of
*   sodium lauryl sulfate in Vaseline (10% w/w) in order to induce local
*   irritation.
**   Day 8: The test site was treated by topical application of the test
*   substance (treated group) or the vehicle (control group) and was covered
*   by an occlusive dressing for 48 hours.
**   Day 22: After a rest period of 12 days, all animals of the treated and
*   control groups were challenged by a topical application of the test
*   substance to the right flank. The left flank served as control and
*   received the vehicle only. Test substance and vehicle were maintained

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*    under an occlusive dressing for 24 hours. Skin reactions were evaluated
*    approximately 24 and 48 hours later.
**
**   At the end of the study, animals were killed without examination of
*    internal organs. No skin samples were taken from the challenge
*    application sites.
**
**   The sensitivity of the guinea pigs was checked with a positive
*    sensitizer: 2,4-dinitro chlorobenzene (DNCB). During the induction
*    period, the test substance was applied at 0.1 % (w/w) (day 1) and 1 %
*    (w/w) (day 8). For the challenge application, the DNCB was applied to the
*    right flank at a concentration of 0.5% (w/w).
F008 CLGETTS
F012 20
F020 120238
EOR
F002 27
F010 5.3
F004 2
F005 RS
F006 sBA is not a dermal sensitizer in guinea pigs. The sensitivity of the
*    guinea pigs was satisfactory since 50% of the animals showed a positive
*    reaction with positive control sensitizer, DNCB. Scores in control and
*    treated groups after challe
F007 sBA is not a dermal sensitizer in guinea pigs. The sensitivity of the
*    guinea pigs was satisfactory since 50% of the animals showed a positive
*    reaction with positive control sensitizer, DNCB. Scores in control and
*    treated groups after challenge with sBA were 0 at both 24 and 48 hours.
F008 CLGETTS
F012 20
F020 120239
EOR
F002 27
F010 5.3
F004 2
F005 SO
F006 Centre d'Elevage Lebeau, Gambais, France
F007 Centre d'Elevage Lebeau, Gambais, France
F008 CLGETTS
F012 20
F020 120240
EOR
F002 27
F010 5.3
F004 2
F005 TS
F006 sec-Butanol (sBA) 99.87%; ATOFINA Chemicals, Inc,
F007 sec-Butanol (sBA) 99.87%; ATOFINA Chemicals, Inc,
F008 CLGETTS
F012 20
F020 120241
EOR
F002 27
F010 5.4
F004 1
F005 CL
F006 MEK has a low order of toxicity based on the 90-day repeated-dose
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*    exposures.  The NOAEL is 2500 ppm.
F007 MEK has a low order of toxicity based on the 90-day repeated-dose
*    exposures.  The NOAEL is 2500 ppm.
F008 CLGETTS
F012 20
F020 120242
EOR
F002 27
F010 5.4
F004 1
F005 RE
F006 Cavender, F.L., Casey, H.W., Salem, H., Swenberg, J.A., and Gralla, E.J.
*    (1983).  A 90-day vapor inhalation toxicity study of methyl ethyl ketone.
*     Fund. Appl. Toxicol. 3:264-270.
F007 Cavender, F.L., Casey, H.W., Salem, H., Swenberg, J.A., and Gralla, E.J.
*    (1983).  A 90-day vapor inhalation toxicity study of methyl ethyl ketone.
*     Fund. Appl. Toxicol. 3:264-270.
F008 HEDSET
F009 21-10-1992
F012 20
F020 120243
EOR
F002 27
F010 5.4
F004 1
F005 RE
F006 Toxigenics. (1981). 90-Day vapor inhalation study of methyl ethyl ketone
*    in albino rats.  Toxigenics' Study 420-0305.  Toxigenics, Inc., 1800 East
*    Pershing Road, Decatur, IL 62526.
F007 Toxigenics. (1981). 90-Day vapor inhalation study of methyl ethyl ketone
*    in albino rats.  Toxigenics' Study 420-0305.  Toxigenics, Inc., 1800 East
*    Pershing Road, Decatur, IL 62526.
F008 HEDSET
F012 20
F020 120244
EOR
F002 27
F010 5.4
F004 1
F005 RL
F006 1 - Reliable study with restrictions.  Study well documented, meets
*    generally accepted scientific principles, acceptable for assessment.
F007 1 - Reliable study with restrictions.  Study well documented, meets
*    generally accepted scientific principles, acceptable for assessment.
F008 HEDSET
F012 20
F020 120245
EOR
F002 27
F010 5.4
F004 1
F005 RM
F006 An extensive pathologic investigation was conducted and no lesions were
*    found that could be attributed to MEK exposure.  There was no indication
*    that repeated exposure to relatively high levels of MEK had any effect on
*    reproductive tissues.
F007 An extensive pathologic investigation was conducted and no lesions were
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*    found that could be attributed to MEK exposure.  There was no indication
*    that repeated exposure to relatively high levels of MEK had any effect on
*    reproductive tissues.  The examined tissues included testes,
*    epididymides, seminal vesicles, vagina, cervix, uterus, oviducts, and
*    ovaries.
F008 HEDSET
F012 20
F020 120246
EOR
F002 27
F010 5.4
F004 1
F005 RM
F006 Methyl ethyl ketone is metabolically interchangeable with
**   2-butanol.  Approximately 97% of a 2-butanol dose is
**   oxidized to methyl ethyl ketone.
F007 Methyl ethyl ketone is metabolically interchangeable with
**   2-butanol.  Approximately 97% of a 2-butanol dose is
**   oxidized to methyl ethyl ketone.
F008 HEDSET
F009 21-10-1992
F012 20
F020 120247
EOR
F002 27
F010 5.4
F004 1
F005 RM
F006 Purity:  > 99.5%
**   Number/Sex/Dose:  15 (10/sex - principals - for routine pathology and
*    5/sex - dedicated -  for special neuropathology)
**   Vehicle:  None
F007 Purity:  > 99.5%
**   Number/Sex/Dose:  15 (10/sex - principals - for routine pathology and
*    5/sex - dedicated -  for special neuropathology)
**   Vehicle:  None
F008 HEDSET
F012 20
F020 120248
EOR
F002 27
F010 5.4
F004 1
F005 RS
F006 The 90-day exposures had no adverse effect on the clinical health or
*    growth of male or female rats except for a depression of mean body weight
*    in the 5000-ppm exposure group.  No animals died during the study.  No
*    signs of nasal irritation
F007 The 90-day exposures had no adverse effect on the clinical health or
*    growth of male or female rats except for a depression of mean body weight
*    in the 5000-ppm exposure group.  No animals died during the study.  No
*    signs of nasal irritation were observed during the study.  There were no
*    treatment-related effects in food consumption or ophthalmologic studies
*    in any of the rats exposed to MEK vapors. The 5000-ppm animals had a
*    slight but significant increase in liver weight, liver weight/body weight
*    ratio and liver weight/brain weight ratio at the time of necropsy.  Serum
*    glutamic-pyruvic transaminase (SGPT) activity in the 2500-ppm female rats
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*    was elevated while the 5000-ppm female rats exhibited significantly
*    decreased SGPT activity.  In addition, alkaline phosphatase, potassium,
*    and glucose values for the 5000-ppm female rats were increased.  Special
*    neuropathological and routine pathological studies did not reveal any
*    lesions that could be attributed to MEK exposure.
F008 HEDSET
F012 20
F020 120249
EOR
F002 27
F010 5.4
F004 1
F005 SO
F006 EXXON CHEMICAL, Limited  Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F007 EXXON CHEMICAL, Limited  Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 120250
EOR
F002 27
F010 5.4
F004 1
F005 TS
F006 Methyl Ethyl Ketone (MEK)
F007 Methyl Ethyl Ketone (MEK)
F008 CLGETTS
F012 20
F020 120251
EOR
F002 27
F010 5.4
F004 2
F005 CL
F006 sBA (probably through its metabolite methyl-ethyl-ketone) was a potent
*    inducer of P-450 in the kidney and liver.
F007 sBA (probably through its metabolite methyl-ethyl-ketone) was a potent
*    inducer of P-450 in the kidney and liver.
F008 CLGETTS
F012 20
F020 120252
EOR
F002 27
F010 5.4
F004 2
F005 RE
F006 Aarstad K., Zahlsen, K., and Nilsen, O. G. (1985).  Inhalation of
*    butanols: changes in the cytochrome p-450 enzyme system. Arch Toxycol
*    (Suppl) 8:418-421.
F007 Aarstad K., Zahlsen, K., and Nilsen, O. G. (1985).  Inhalation of
*    butanols: changes in the cytochrome p-450 enzyme system. Arch Toxycol
*    (Suppl) 8:418-421.
F008 CLGETTS
F012 20
F020 120253
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EOR
F002 27
F010 5.4
F004 2
F005 RL
F006 2- Reliable study with restrictions. Study well documented, meets
*   generally accepted scientific principles, acceptable for assessment.
F007 2- Reliable study with restrictions. Study well documented, meets
*   generally accepted scientific principles, acceptable for assessment.
F008 CLGETTS
F012 20
F020 120254
EOR
F002 27
F010 5.4
F004 2
F005 RM
F006 Purity: > or = 99%
**   Number/Sex/Dose: 5
**   Vehicle: None
F007 Purity: > or = 99%
**   Number/Sex/Dose: 5
**   Vehicle: None
F008 CLGETTS
F012 20
F020 120255
EOR
F002 27
F010 5.4
F004 2
F005 RS
F006 sBA caused increases in cytochrome P-450 concentrations in the kidneys
*   (47% rise; 500 ppm for 5 days) and liver (33% rise; 2000 ppm for 3 days).
*   Slight decreases in lung cytochrome P-450 were observed.
F007 sBA caused increases in cytochrome P-450 concentrations in the kidneys
*   (47% rise; 500 ppm for 5 days) and liver (33% rise; 2000 ppm for 3 days).
*   Slight decreases in lung cytochrome P-450 were observed.
F008 CLGETTS
F012 20
F020 120256
EOR
F002 27
F010 5.5
F004 1
F005 CL
F006 Not Mutagenic
F007 Not Mutagenic
F008 CLGETTS
F012 20
F020 120257
EOR
F002 27
F010 5.5
F004 1
F005 RE
F006 Brooks, T. M., Meyer, A., and Hutson, D. H. (1988). The genetic
*   toxicology of some hydrocarbon and oxygenated solvents. Mutagenesis,

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*    3(3):227-231.
F007 Brooks, T. M., Meyer, A., and Hutson, D. H. (1988).  The genetic
*    toxicology of some hydrocarbon and oxygenated solvents.  Mutagenesis,
*    3(3):227-231.
F008 CLGETTS
F012 20
F020 120258
EOR
F002 27
F010 5.5
F004 1
F005 RL
F006 1- Reliable without restriction
F007 1- Reliable without restriction
F008 CLGETTS
F012 20
F020 120259
EOR
F002 27
F010 5.5
F004 1
F005 RM
F006 Purity:  99.5%
**   Strain:  S. typhimurium / TA98, TA100, TA1535, TA1537, TA1538
**   Species/Cell Type:  Rat Liver (S9 fraction)
**   Vehicle:  DMSO
F007 Purity:  99.5%
**   Strain:  S. typhimurium / TA98, TA100, TA1535, TA1537, TA1538
**   Species/Cell Type:  Rat Liver (S9 fraction)
**   Vehicle:  DMSO
F008 CLGETTS
F012 20
F020 120260
EOR
F002 27
F010 5.5
F004 1
F005 RM
F006 sBA did not induce reverse gene mutation in bacteria.
F007 sBA did not induce reverse gene mutation in bacteria.
F008 CLGETTS
F012 20
F020 120261
EOR
F002 27
F010 5.5
F004 1
F005 SO
F006 EXXON CHEMICAL, Limited  Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F007 EXXON CHEMICAL, Limited  Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 120262
EOR
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F002 27
F010 5.5
F004 1
F005 TC
F006 Control plates were set up with solvent alone and with an appropriate
*   known positive control compound. All tests were carried out in
*   triplicate. Two replicate assays were carried on different days in order
*   to confirm the reproducibility o
F007 Control plates were set up with solvent alone and with an appropriate
*   known positive control compound. All tests were carried out in
*   triplicate. Two replicate assays were carried on different days in order
*   to confirm the reproducibility of the results. The S9 fractions were
*   prepared from Aroclor-induced rats. Initially, a range of test
*   concentrations of test material was tested and a second experiment was
*   then performed based on the results taking into account the effect on
*   cell viability and any possible positive increases in mitotic gene
*   conversion. Control plates were set up with solvent alone and with the
*   positive control compounds 4-nitroquinoline-N-oxide and cyclophosphamide.
F008 CLGETTS
F012 20
F020 120263
EOR
F002 27
F010 5.5
F004 2
F005 CL
F006 Not Mutagenic
F007 Not Mutagenic
F008 CLGETTS
F012 20
F020 120264
EOR
F002 27
F010 5.5
F004 2
F005 RE
F006 Brooks, T. M., Meyer, A., and Hutson, D. H. (1988). The genetic
*   toxicology of some hydrocarbon and oxygenated solvents. Mutagenesis,
*   3(3):227-231.
F007 Brooks, T. M., Meyer, A., and Hutson, D. H. (1988). The genetic
*   toxicology of some hydrocarbon and oxygenated solvents. Mutagenesis,
*   3(3):227-231.
F008 CLGETTS
F012 20
F020 120265
EOR
F002 27
F010 5.5
F004 2
F005 RL
F006 1- Reliable without restriction.
F007 1- Reliable without restriction.
F008 CLGETTS
F012 20
F020 120266
EOR
F002 27

F010 5.5
F004 2
F005 RM
F006 Purity: 99.5%
**   Strain: E. coli WP2 uvr A
**   Species/Cell Type: Rat Liver (S9 fraction)
**   Vehicle: DMSO
F007 Purity: 99.5%
**   Strain: E. coli WP2 uvr A
**   Species/Cell Type: Rat Liver (S9 fraction)
**   Vehicle: DMSO
F008 CLGETTS
F012 20
F020 120267
EOR
F002 27
F010 5.5
F004 2
F005 RM
F006 sBA did not induce reverse gene mutation in bacteria.
F007 sBA did not induce reverse gene mutation in bacteria.
F008 CLGETTS
F012 20
F020 120268
EOR
F002 27
F010 5.5
F004 2
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 120269
EOR
F002 27
F010 5.5
F004 2
F005 TC
F006 Control plates were set up with solvent alone and with an appropriate
*   known positive control compound. All tests were carried out in
*   triplicate. Two replicate assays were carried on different days in order
*   to confirm the reproducibility o
F007 Control plates were set up with solvent alone and with an appropriate
*   known positive control compound. All tests were carried out in
*   triplicate. Two replicate assays were carried on different days in order
*   to confirm the reproducibility of the results. The S9 fractions were
*   prepared from Aroclor-induced rats. Initially, a range of test
*   concentrations of test material was tested and a second experiment was
*   then performed based on the results taking into account the effect on
*   cell viability and any possible positive increases in mitotic gene
*   conversion. Control plates were set up with solvent alone and with the
*   positive control compounds 4-nitroquinoline-N-oxide and cyclophosphamide.
F008 CLGETTS

F012 20
F020 120270
EOR
F002 27
F010 5.5
F004 3
F005 CL
F006 Not mutagenic
F007 Not mutagenic
F008 CLGETTS
F012 20
F020 120271
EOR
F002 27
F010 5.5
F004 3
F005 RE
F006 Brooks, T. M., Meyer, A., and Hutson, D. H. (1988). The genetic
*   toxicology of some hydrocarbon and oxygenated solvents. Mutagenesis,
*   3(3):227-231.
F007 Brooks, T. M., Meyer, A., and Hutson, D. H. (1988). The genetic
*   toxicology of some hydrocarbon and oxygenated solvents. Mutagenesis,
*   3(3):227-231.
F008 CLGETTS
F012 20
F020 120272
EOR
F002 27
F010 5.5
F004 3
F005 RL
F006 1- Reliable without restriction
F007 1- Reliable without restriction
F008 CLGETTS
F012 20
F020 120273
EOR
F002 27
F010 5.5
F004 3
F005 RM
F006 Purity: 99.5%
**   Strain: Saccharomyces cerevisiae
**   Species/Cell Type: Rat Liver (S9 fraction)
**   Vehicle: DMSO
F007 Purity: 99.5%
**   Strain: Saccharomyces cerevisiae
**   Species/Cell Type: Rat Liver (S9 fraction)
**   Vehicle: DMSO
F008 CLGETTS
F012 20
F020 120274
EOR
F002 27
F010 5.5
F004 3
F005 RM

F006 sBA did not induce mitotic gene conversion in yeast.
F007 sBA did not induce mitotic gene conversion in yeast.
F008 CLGETTS
F012 20
F020 120275
EOR
F002 27
F010 5.5
F004 3
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
** EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
** EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 120276
EOR
F002 27
F010 5.5
F004 3
F005 TC
F006 Yeast cells were grown in log phase, washed and re-suspended in 2/5
* strength YEPD broth at a concentration of 10 X 106cells/ml. The
* suspension was then divided into 1.9 ml amounts in 30-ml universal
* containers and 0.1 ml of the test compou
F007 Yeast cells were grown in log phase, washed and re-suspended in 2/5
* strength YEPD broth at a concentration of 10 X 106cells/ml. The
* suspension was then divided into 1.9 ml amounts in 30-ml universal
* containers and 0.1 ml of the test compound solution was added (-S9). For
* the experiments with metabolic activation (+S9), 0.1 ml of the compound
* was added to 1.6 ml of yeast suspension, together with 0.3 ml of S9 mix.
* The cultures were incubated with shaking, with shaking, at 30°C for 18
* hours. Aliquots were then plated onto the appropriate culture media for
* the selection of mitotic gene convertants and cells surviving the
* treatment.
F008 CLGETTS
F012 20
F020 120277
EOR
F002 27
F010 5.5
F004 4
F005 CL
F006 Not Mutagenic
F007 Not Mutagenic
F008 CLGETTS
F012 20
F020 120278
EOR
F002 27
F010 5.5
F004 4
F005 RE
F006 Brooks, T. M., Meyer, A., and Hutson, D. H. (1988). The genetic
* toxicology of some hydrocarbon and oxygenated solvents. Mutagenesis,

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*    3(3):227-231.
F007 Brooks, T. M., Meyer, A., and Hutson,  D. H. (1988).  The genetic
*    toxicology of some hydrocarbon and oxygenated solvents.  Mutagenesis,
*    3(3):227-231.
F008 HEDSET
F009 21-10-1992
F012 20
F020 120279
EOR
F002 27
F010 5.5
F004 4
F005 RL
F006 1- Reliable without restriction
F007 1- Reliable without restriction
F008 HEDSET
F012 20
F020 120280
EOR
F002 27
F010 5.5
F004 4
F005 RM
F006 Purity:  99.5%
**   Species/Cell Type:  Chinese Hamster Ovary Cells
**   Vehicle:  DMSO
F007 Purity:  99.5%
**   Species/Cell Type:  Chinese Hamster Ovary Cells
**   Vehicle:  DMSO
F008 HEDSET
F012 20
F020 120281
EOR
F002 27
F010 5.5
F004 4
F005 RM
F006 sBA did not induce chromosome damage in CHO mammalian cells.
F007 sBA did not induce chromosome damage in CHO mammalian cells.
F008 HEDSET
F012 20
F020 120282
EOR
F002 27
F010 5.5
F004 4
F005 RS
F006 Negative - No increase in chromosomal aberrations
F007 Negative - No increase in chromosomal aberrations
F008 HEDSET
F012 20
F020 120283
EOR
F002 27
F010 5.5
F004 4
F005 SO
```

F006 EXXON CHEMICAL, Limited Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 120284
EOR
F002 27
F010 5.5
F004 4
F005 TC
F006 Two separate cytotoxicity assays were performed: (i) Monolayer CHO
*   cultures were prepared in multi-well tissue culture trays. The cultures
*   were incubated at 37°C for 24 hours to commence active growth before
*   treatment with the test materia
F007 Two separate cytotoxicity assays were performed: (i) Monolayer CHO
*   cultures were prepared in multi-well tissue culture trays. The cultures
*   were incubated at 37°C for 24 hours to commence active growth before
*   treatment with the test material. Assays were performed both in the
*   presence and in the absence of S9 mix using either a 5-hour exposure
*   (+S9) or a 24-hour exposure (-S9). Twenty-four hours after initial
*   treatment, cultures were stained with Giemsa and the growth inhibition
*   was noted. (ii) CHO cultures were prepared in 25 cm2 flasks, and after
*   24 hours the cells were exposed to sBA both in the presence and in the
*   absence of S9 mix. The number of cell in each flask was counted 24 hours
*   later. The compound concentrations selected for the chromosome assays
*   were 1, 0.5, and 0.25 times the GI50 level.
**
**   CHO Chromosome Assay: Cultured CHO cells were grown in 80-cm2 flasks for
*   24 hours before treatment. Treatment periods were 5hours in the presence
*   of S9 mix and 24 hours in the absence of S9 mix. Positive control
*   cultures were run in parallel [ethyl methanesulphonate (-S9) and
*   cyclophosphamide (+S9). Colcemid was added to all cultures 22 hours after
*   treatment. After a further 2 hours, the cells were trypsinized,
*   resuspended in hypotonic solution and then fixative, before spotting onto
*   slides. Cell preparations were then stained with Giemsa. The slides
*   were randomly coded and 100 cells from each culture were analyzed
*   microscopically. Mitotic index estimations were also made.
F008 CLGETTS
F012 20
F020 120285
EOR
F002 27
F010 5.5
F004 5
F005 CL
F006 Not Mutagenic
F007 Not Mutagenic
F008 CLGETTS
F012 20
F020 120286
EOR
F002 27
F010 5.5
F004 5

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F005 RE
F006 ELF ATOCHEM, BUTANOL SECONDAIRE TEST DE AMES "essai de mutation reverse
*    sur Salmonella typhirium" SANOFI RECHERCHE Report CEL357A/C, 1989.
F007 ELF ATOCHEM, BUTANOL SECONDAIRE TEST DE AMES "essai de mutation reverse
*    sur Salmonella typhirium" SANOFI RECHERCHE Report CEL357A/C, 1989.
F008 HEDSET
F009 02-06-1994
F012 20
F020 120287
EOR
F002 27
F010 5.5
F004 5
F005 RL
F006 1- Reliable without restriction
F007 1- Reliable without restriction
F008 HEDSET
F012 20
F020 120288
EOR
F002 27
F010 5.5
F004 5
F005 RM
F006 sBA did not induce reverse gene mutation in bacteria.
F007 sBA did not induce reverse gene mutation in bacteria.
F008 HEDSET
F012 20
F020 120289
EOR
F002 27
F010 5.5
F004 5
F005 RM
F006 Strain:  Salmonella typhimurium / TA98, TA100, TA1535, TA1537, TA1538
**   Species/Cell Type:  Rat Liver (S9 fraction)
**   Vehicle:  DMSO
F007 Strain:  Salmonella typhimurium / TA98, TA100, TA1535, TA1537, TA1538
**   Species/Cell Type:  Rat Liver (S9 fraction)
**   Vehicle:  DMSO
F008 HEDSET
F012 20
F020 120290
EOR
F002 27
F010 5.5
F004 5
F005 SO
F006 EXXON CHEMICAL, Limited  Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F007 EXXON CHEMICAL, Limited  Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 120291
EOR
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F002 27
F010 5.5
F004 5
F005 TC
F006 Control plates were set up with solvent alone and with an appropriate
*   known positive control compound. All tests were carried out in
*   triplicate. Two replicate assays were carried out on different days in
*   order to confirm the reproducibili
F007 Control plates were set up with solvent alone and with an appropriate
*   known positive control compound. All tests were carried out in
*   triplicate. Two replicate assays were carried out on different days in
*   order to confirm the reproducibility of the results. The S9 fractions
*   were prepared from Aroclor -induced rats. Initially, a range of test
*   concentrations of test material was tested and a second experiment was
*   then performed based on the results taking into account the effect on
*   cell viability and any possible positive increases in mitotic gene
*   conversion. Control plates were set up with solvent alone and with the
*   positive control compounds 4-nitroquinoline-N-oxide and cyclophosphamide.
F008 CLGETTS
F012 20
F020 120292
EOR
F002 27
F010 5.6
F004 1
F005 CL
F006 unknown
F007 unknown
F008 CLGETTS
F012 20
F020 120293
EOR
F002 27
F010 5.6
F004 1
F005 RE
F006 Barilyak, I. R. and Kozachuk, SYu. (1988). Investigation of the
*   cytogenetic effect of a number of monohydric alcohols on rat bone marrow
*   cells. Cytology and Genetics (Tsitologiaya I Genetika), 22(2):49-52.
F007 Barilyak, I. R. and Kozachuk, SYu. (1988). Investigation of the
*   cytogenetic effect of a number of monohydric alcohols on rat bone marrow
*   cells. Cytology and Genetics (Tsitologiaya I Genetika), 22(2):49-52.
F008 CLGETTS
F012 20
F020 120294
EOR
F002 27
F010 5.6
F004 1
F005 RL
F006 4 - Incomplete translation from Russian and insufficient for assessment
F007 4 - Incomplete translation from Russian and insufficient for assessment
F008 CLGETTS
F012 20
F020 120295
EOR
F002 27

F010 5.6
F004 1
F005 RM
F006 Single intragastric administration of monohydric alcohols at equitoxic
*   doses (1/5 LD50) affected the chromosomal appearance of bone marrow.
F007 Single intragastric administration of monohydric alcohols at equitoxic
*   doses (1/5 LD50) affected the chromosomal appearance of bone marrow.
F008 CLGETTS
F012 20
F020 120296
EOR
F002 27
F010 5.6
F004 1
F005 RM
F006 System of Testing: Rat Bone Marrow
**   Metabolic Activation: unknown
**   Species/Cell Type: Rat
**   Concentrations Tested: 1/5 of the LD50 by intragastric route
**   Vehicle: unknown
F007 System of Testing: Rat Bone Marrow
**   Metabolic Activation: unknown
**   Species/Cell Type: Rat
**   Concentrations Tested: 1/5 of the LD50 by intragastric route
**   Vehicle: unknown
F008 CLGETTS
F012 20
F020 120297
EOR
F002 27
F010 5.6
F004 1
F005 RS
F006 Increased numbers of polyploid cells, cells with chromosome gaps, and
*   cells with chromosomal aberrations.
F007 Increased numbers of polyploid cells, cells with chromosome gaps, and
*   cells with chromosomal aberrations.
F008 CLGETTS
F012 20
F020 120298
EOR
F002 27
F010 5.6
F004 2
F005 CL
F006 MEK did not induce a statistically significant increase in the mean
*   number of micronucleated polychromatic erythrocytes in the bone marrow of
*   CD-1 mice. Therefore, it is not considered mutagenic under the
*   conditions of this assay.
F007 MEK did not induce a statistically significant increase in the mean
*   number of micronucleated polychromatic erythrocytes in the bone marrow of
*   CD-1 mice. Therefore, it is not considered mutagenic under the
*   conditions of this assay.
F008 CLGETTS
F012 20
F020 120299
EOR

F002 27
F010 5.6
F004 2
F005 RE
F006 O'Donoghue, J.L., Haworth, S.R., Curren, R.D., Kirby, P.E., Lawlor, T.,
*   Moran, E.J., Phillips, R.D., Putnam, D.L., Rogers-Back, A.M., Slesinski,
*   R.S., and Thilagar, A. (1988). Mutagenicity studies on ketone solvents:
*   methyl ethyl ketone, me
F007 O'Donoghue, J.L., Haworth, S.R., Curren, R.D., Kirby, P.E., Lawlor, T.,
*   Moran, E.J., Phillips, R.D., Putnam, D.L., Rogers-Back, A.M., Slesinski,
*   R.S., and Thilagar, A. (1988). Mutagenicity studies on ketone solvents:
*   methyl ethyl ketone, methyl isobutyl ketone, and isophorone. Mutation
*   Research, 206:149-161.
F008 CLGETTS
F012 20
F020 120300
EOR
F002 27
F010 5.6
F004 2
F005 RL
F006 1 - Reliable without Restrictions. No circumstances occurred that would
*   have affected the quality or integrity of the data.
F007 1 - Reliable without Restrictions. No circumstances occurred that would
*   have affected the quality or integrity of the data.
F008 CLGETTS
F012 20
F020 120301
EOR
F002 27
F010 5.6
F004 2
F005 RM
F006 Not mutagenic
F007 Not mutagenic
F008 CLGETTS
F012 20
F020 120302
EOR
F002 27
F010 5.6
F004 2
F005 RM
F006 Purity: 99.9%
**   Number: 5/sex/dose
**   Dose/Time: 1.96 ml/kg Single injection (dose equal to the MEK LD20
*   reported as ml test article / kg body weight when administered in a total
*   volume of 10 ml test article-vehicle mixture / kg body weight).
F007 Purity: 99.9%
**   Number: 5/sex/dose
**   Dose/Time: 1.96 ml/kg Single injection (dose equal to the MEK LD20
*   reported as ml test article / kg body weight when administered in a total
*   volume of 10 ml test article-vehicle mixture / kg body weight).
**   Vehicle: Corn Oil (10 ml/kg)
**   Positive Control: 0.25 mg/kg Triethylene melamine (TEM)
F008 CLGETTS
F012 20

F020 120303
EOR
F002 27
F010 5.6
F004 2
F005 RM
F006 The test substance and the vehicle were administered as a single dose by
*   intraperitoneal injection. The vehicle was dosed at a volume equal to
*   the test substance volume. The positive control was administered as a
*   single dose at a volume e
F007 The test substance and the vehicle were administered as a single dose by
*   intraperitoneal injection. The vehicle was dosed at a volume equal to
*   the test substance volume. The positive control was administered as a
*   single dose at a volume equal to the test substance volume. Animals from
*   the appropriate groups were sacrificed at approximately 12, 24 and 48
*   hours. Animals dosed with triethylene melamine were sacrificed at 24
*   hours only. Immediately following sacrifice, the femur was exposed and
*   the bone marrow was aspirated into a syringe containing fetal calf serum.
*   The cells were washed, centrifuged, and resuspended. Slide smears of
*   the bone marrow were made for each animal and stained with
*   May-Gruenwald-Giemsa stain. Coded slides were then evaluated for
*   presence of micronuclei (1000 polychromatic erythrocytes/animal were
*   evaluated). A 1-way analysis of variance and Duncan's multiple range
*   test (p = 0.05) were used to assess the statistical significance of any
*   observed effects.
F008 CLGETTS
F012 20
F020 120304
EOR
F002 27
F010 5.6
F004 2
F005 RS
F006 None of the dose groups were statistically different from the vehicle
*   control. The positive control (0.25 mg/kg TEM) induced a statistically
*   significant increase in the mean number of micronucleated polychromatic
*   erythrocytes (p = 0.01) wh
F007 None of the dose groups were statistically different from the vehicle
*   control. The positive control (0.25 mg/kg TEM) induced a statistically
*   significant increase in the mean number of micronucleated polychromatic
*   erythrocytes (p = 0.01) which indicates that the positive control was
*   clastogenic and the test system responded in an appropriate manner.
*   Vehicle carrier control values for the mean percent of polychromatic
*   erythrocytes and for the mean percent of micronucleated polychromatic
*   erythrocytes responded in an appropriate manner.
F008 CLGETTS
F012 20
F020 120305
EOR
F002 27
F010 5.6
F004 2
F005 TS
F006 Methyl Ethyl Ketone (MEK) CAS No. 78-93-3
F007 Methyl Ethyl Ketone (MEK) CAS No. 78-93-3
F008 CLGETTS
F012 20

F020 120306
EOR
F002 27
F010 5.7
F004 1
F005 RM
F006 No studies of 2-butanol for carcinogenic activity have been
** reported; however, based on results of mutagenicity assays
** it is expected to have a low potential for carcinogenicity.
F007 No studies of 2-butanol for carcinogenic activity have been
** reported; however, based on results of mutagenicity assays
** it is expected to have a low potential for carcinogenicity.
F008 HEDSET
F009 21-10-1992
F012 20
F020 120307
EOR
F002 27
F010 5.7
F004 1
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
** EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
** EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 120308
EOR
F002 27
F010 5.8.1
F004 1
F005 CL
F006 sBA is not a reproductive hazard.
F007 sBA is not a reproductive hazard.
F008 CLGETTS
F012 20
F020 120309
EOR
F002 27
F010 5.8.1
F004 1
F005 RE
F006 Cox, G.E., D.E. Bailey and K. Morgareidge. (1975). Toxicity studies in
* rats with 2-butanol including growth, reproduction and teratologic
* observations. LaB No. 2093. Food and Drug Research Laboratories, Inc.,
* Waverly, NY.
F007 Cox, G.E., D.E. Bailey and K. Morgareidge. (1975). Toxicity studies in
* rats with 2-butanol including growth, reproduction and teratologic
* observations. LaB No. 2093. Food and Drug Research Laboratories, Inc.,
* Waverly, NY.
F008 HEDSET
F009 31-03-1994
F012 20
F020 120310
EOR

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F002 27
F010 5.8.1
F004 1
F005 RE
F006 Gallo, M.A., Oser, B.L., Cox, G.E., and Bailey, D.E. (1977). Studies on
*    the long-term toxicity of 2-butanol. Toxicology and Applied Pharmacology,
*    41:135 (Abstract).
F007 Gallo, M.A., Oser, B.L., Cox, G.E., and Bailey, D.E. (1977). Studies on
*    the long-term toxicity of 2-butanol. Toxicology and Applied Pharmacology,
*    41:135 (Abstract).
F008 HEDSET
F012 20
F020 120311
EOR
F002 27
F010 5.8.1
F004 1
F005 RL
F006 2 - Reliable study with restrictions.  No circumstances occurred that
*    would have affected the quality or integrity of the data. Comparable to a
*    guideline study and test procedures were in accordance with generally
*    accepted scientific standa
F007 2 - Reliable study with restrictions.  No circumstances occurred that
*    would have affected the quality or integrity of the data. Comparable to a
*    guideline study and test procedures were in accordance with generally
*    accepted scientific standards and described in sufficient detail.
F008 HEDSET
F012 20
F020 120312
EOR
F002 27
F010 5.8.1
F004 1
F005 RM
F006 Purity:  > or = 99%
**
**   Number/Sex/Dose:  30
**
**   Doses/Concentration:
**   F0 Generation: 0, 0.3, 1.0, or 3.0% solutions (0, 538, 1644, and 5089
*    mg/kg-day for males and 0, 594, 1771, and 4571 mg/kg-day for females)
**   F1 Generation: 0, 0.3, 1.0, or 2.0%
F007 Purity:  > or = 99%
**
**   Number/Sex/Dose:  30
**
**   Doses/Concentration:
**   F0 Generation: 0, 0.3, 1.0, or 3.0% solutions (0, 538, 1644, and 5089
*    mg/kg-day for males and 0, 594, 1771, and 4571 mg/kg-day for females)
**   F1 Generation: 0, 0.3, 1.0, or 2.0% (2.0% calculated to be equivalent to
*    3384 mg/kg-day for males and 3122 mg/kg-day for females)
**
**   Vehicle:  Drinking Water
F008 HEDSET
F012 20
F020 120313
EOR
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F002 27
F010 5.8.1
F004 1
F005 RM
F006 sec-Butanol was initially administered to the F0 generation at
*   concentrations of 0, 0.3, 1.0, and 3.0% in the drinking water. Due to
*   toxicity, the high level was reduced to 2.0% during the second-generation
*   study (F1). The F1 generation a
F007 sec-Butanol was initially administered to the F0 generation at
*   concentrations of 0, 0.3, 1.0, and 3.0% in the drinking water. Due to
*   toxicity, the high level was reduced to 2.0% during the second-generation
*   study (F1). The F1 generation animals (30/sex/group) were reared to
*   maturity (up to week 12), mated to produce a F2 generation, then
*   sacrificed for organ weights, and gross and microscopic pathological
*   evaluations (10/sex/group). Hematological, biochemical, and urinary
*   examinations were conducted terminally on the F1 rats. A series of mild
*   changes in the kidney (non-reactive tubular degeneration, tubular casts,
*   foci of tubular regeneration, microcysts) were observed animals treated
*   at 2.0% sBA. The authors concluded that these findings were not a result
*   of direct toxicity and did not have clear pathologic significance.
*   Rather they were non-specific effects due to increased renal work load,
*   possibly from increased urine volume and pressure at the high dose of sBA
*   (Cox et al, 1975). No other findings of note were seen. The no-effect
*   level for the study was 1.0% (estimated to be 1500 mg/kg/day by the
*   authors and 1771 mg/kg/day by EPA/IRIS).
F008 HEDSET
F012 20
F020 120314
EOR
F002 27
F010 5.8.1
F004 1
F005 RS
F006 Maternal NOEL: 1% (~1500 mg/kg/day)
**   Maternal NOAEL: 1771 mg/kg/day
**   Pup NOEL: 1% (~1500 mg/kg/day)
**   Pup NOAEL: 1771 mg/kg/day
F007 Maternal NOEL: 1% (~1500 mg/kg/day)
**   Maternal NOAEL: 1771 mg/kg/day
**   Pup NOEL: 1% (~1500 mg/kg/day)
**   Pup NOAEL: 1771 mg/kg/day
F008 HEDSET
F012 20
F020 120315
EOR
F002 27
F010 5.8.1
F004 1
F005 SO
F006 EXXON CHEMICAL, Limited Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F007 EXXON CHEMICAL, Limited Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 120316

EOR
F002 27
F010 5.8.2
F004 1
F005 CL
F006 sBA is not a teratogen. There was no evidence of teratogenic events nor
*   was there evidence of selective developmental toxicity.
F007 sBA is not a teratogen. There was no evidence of teratogenic events nor
*   was there evidence of selective developmental toxicity.
F008 CLGETTS
F012 20
F020 120317
EOR
F002 27
F010 5.8.2
F004 1
F005 ME
F006 For the maternal data, multivariate analysis (with baseline as covariant)
*   was used for weight comparisons across groups. The group differences in
*   food and water intake were analyzed by multivariate analysis of variance.
*   A Kruskal-Wallis te
F007 For the maternal data, multivariate analysis (with baseline as covariant)
*   was used for weight comparisons across groups. The group differences in
*   food and water intake were analyzed by multivariate analysis of variance.
*   A Kruskal-Wallis test was used for group comparisons of corpora lutea
*   per animal. For the fetal data, analysis of covariance was used to
*   compare fetal weights across groups and sex. Group comparisons of the
*   variables including litter size, percentage alive/litter, percentage
*   normal/litter, and percentage females/litter were made using
*   Kruskal-Wallis test. For the variables including skeletal malformations,
*   skeletal variations, visceral malformations, visceral variations,
*   external malformations, and non-normal fetuses, the number of litters
*   with one or more of the variables of interest was compared between groups
*   using Fisher's exact test. The results of the test were adjusted for
*   multiple comparisons, when appropriate, using the Bonferroni technique.
*   A probability of p = < 0.05 was required for significance.
F008 CLGETTS
F012 20
F020 120318
EOR
F002 27
F010 5.8.2
F004 1
F005 RE
F006 Nelson, B. K., Brightwell, W. S., Khan, A., Burg, J. R., and Goad, P. T.
*   (1989). Lack of selective developmental toxicity of three butanol
*   isomers administered by inhalation to rats. Fundam Appl Toxicol,
*   12:469-479.
F007 Nelson, B. K., Brightwell, W. S., Khan, A., Burg, J. R., and Goad, P. T.
*   (1989). Lack of selective developmental toxicity of three butanol
*   isomers administered by inhalation to rats. Fundam Appl Toxicol,
*   12:469-479.
F008 HEDSET
F009 21-10-1992
F012 20
F020 120319
EOR

F002 27
F010 5.8.2
F004 1
F005 RL
F006 2- Reliable study with restrictions. Study well documented, meets
*   generally accepted scientific principles, acceptable for assessment.
F007 2- Reliable study with restrictions. Study well documented, meets
*   generally accepted scientific principles, acceptable for assessment.
F008 HEDSET
F012 20
F020 120320
EOR
F002 27
F010 5.8.2
F004 1
F005 RM
F006 Groups of 15-16 rats were exposed by inhalation to 0, 3,500, 5,000 or
*   7,000 ppm sBA, 7 hours/day on days 1-19 of gestation; the dams were
*   sacrificed on day 20. At 7,000 ppm, narcosis was observed in all
*   animals. At 5000 ppm, the dams were
F007 Groups of 15-16 rats were exposed by inhalation to 0, 3,500, 5,000 or
*   7,000 ppm sBA, 7 hours/day on days 1-19 of gestation; the dams were
*   sacrificed on day 20. At 7,000 ppm, narcosis was observed in all
*   animals. At 5000 ppm, the dams were partially narcotized with locomotion
*   activity impaired. Maternal weight gain and food consumption were
*   significantly reduced in all dose groups. No data collected on maternal
*   organ weights, or gross or microscopic lesions. The number of live
*   fetuses was significantly reduced and resorptions were increased in the
*   high exposure group only. Fetal body weights were significantly reduced
*   in the mid- and high dose groups. There was no evidence of teratogenic
*   effects in this study, and there was also no evidence of selective
*   developmental toxicity. The no-effect levels were < 3,500 ppm for
*   maternal toxicity and 3,500 ppm for developmental toxicity.
F008 HEDSET
F012 20
F020 120321
EOR
F002 27
F010 5.8.2
F004 1
F005 RM
F006 Purity: > or = 99%
**   Number/Sex/Dose: 15-16 Mated Females
**   Vehicle: None
F007 Purity: > or = 99%
**   Number/Sex/Dose: 15-16 Mated Females
**   Vehicle: None
F008 HEDSET
F012 20
F020 120322
EOR
F002 27
F010 5.8.2
F004 1
F005 RS
F006 Maternal NOEL: < 3500 ppm
**   Maternal NOAEL: 3500 ppm

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**   Pup NOEL:  3500 ppm
**   Pup NOAEL:  > 7000 ppm
F007 Maternal NOEL:  < 3500 ppm
**   Maternal NOAEL:  3500 ppm
**   Pup NOEL:  3500 ppm
**   Pup NOAEL:  > 7000 ppm
F008 HEDSET
F012 20
F020 120323
EOR
F002 27
F010 5.8.2
F004 1
F005 SO
F006 EXXON CHEMICAL, Limited  Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F007 EXXON CHEMICAL, Limited  Fareham, Hampshire
**   EUROPEAN COMMISSION - European Chemicals Bureau  Ispra (VA)
F008 CLGETTS
F009 09-01-2002
F012 20
F020 120324
EOR
F002 27
F010 5.8.2
F004 2
F005 CL
F006 Not a teratogen.
F007 Not a teratogen.
F008 CLGETTS
F012 20
F020 120325
EOR
F002 27
F010 5.8.2
F004 2
F005 RE
F006 Cox, G.E., D.E. Bailey and K. Morgareidge. (1975). Toxicity studies in
*    rats with 2-butanol including growth, reproduction and teratologic
*    observations. LaB No. 2093. Food and Drug Research Laboratories, Inc.,
*    Waverly, NY.
F007 Cox, G.E., D.E. Bailey and K. Morgareidge. (1975). Toxicity studies in
*    rats with 2-butanol including growth, reproduction and teratologic
*    observations. LaB No. 2093. Food and Drug Research Laboratories, Inc.,
*    Waverly, NY.
F008 CLGETTS
F012 20
F020 120326
EOR
F002 27
F010 5.8.2
F004 2
F005 RE
F006 Gallo, M.A., Oser, B.L., Cox, G.E., and Bailey, D.E. (1977). Studies on
*    the long-term toxicity of 2-butanol. Toxicology and Applied Pharmacology,
*    41:135 (Abstract).
F007 Gallo, M.A., Oser, B.L., Cox, G.E., and Bailey, D.E. (1977). Studies on
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*    the long-term toxicity of 2-butanol. Toxicology and Applied Pharmacology,
*    41:135 (Abstract).
F008 CLGETTS
F012 20
F020 120327
EOR
F002 27
F010 5.8.2
F004 2
F005 RL
F006 2 - Reliable study with restrictions.  No circumstances occurred that
*    would have affected the quality or integrity of the data. Comparable to a
*    guideline study and test procedures were in accordance with generally
*    accepted scientific standa
F007 2 - Reliable study with restrictions.  No circumstances occurred that
*    would have affected the quality or integrity of the data. Comparable to a
*    guideline study and test procedures were in accordance with generally
*    accepted scientific standards and described in sufficient detail.
F008 CLGETTS
F012 20
F020 120328
EOR
F002 27
F010 5.8.2
F004 2
F005 RM
F006 Purity:  > or = 99%
**   Doses/Concentration:  F0 Generation - second breeding.
**   0, 0.3, 1.0, or 2.0% solutions (0, 538, 1644, and 3384 mg/kg-day for
*    males and 0, 594, 1771, and 3122 mg/kg-day for females)
**   Vehicle:  Drinking Water
**   Number/Sex/Dose
F007 Purity:  > or = 99%
**   Doses/Concentration:  F0 Generation - second breeding.
**   0, 0.3, 1.0, or 2.0% solutions (0, 538, 1644, and 3384 mg/kg-day for
*    males and 0, 594, 1771, and 3122 mg/kg-day for females)
**   Vehicle:  Drinking Water
**   Number/Sex/Dose:  30
F008 CLGETTS
F012 20
F020 120329
EOR
F002 27
F010 5.8.2
F004 2
F005 RM
F006 TERATOLOGY SCREEN RESULT: The F0 rats were mated to obtain a second
*    series of pregnant dams destined to provide teratologic evaluation of the
*    treatments.  Pregnancy rates and survival of these females were
*    unaffected. All findings sBA at bo
F007 TERATOLOGY SCREEN RESULT: The F0 rats were mated to obtain a second
*    series of pregnant dams destined to provide teratologic evaluation of the
*    treatments.  Pregnancy rates and survival of these females were
*    unaffected. All findings sBA at both 0.3 and 1.0% in the drinking water
*    were negative with respect to signs of toxicity in terms of both growth
*    and reproductive efficiency The body weights of the dams were not
*    depressed. Examination of the uterine contents on the 20th day of
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*    gestation revealed that sBA was somewhat fetotoxic at the 2.0% dosage
*    level, as shown by the decreased pup weights (3.74 g vs. 4.14 g in
*    controls). However, that this is a minimal response is shown by the fact
*    that none of the other parameters in the reproductive toxicity phase of
*    this study (nidation, early or late fetal deaths) were affected. The 2.0%
*    group showed apparent increases in missing sternebrae, wavy ribs, and
*    incomplete vertebra ossification when compared with both the 0.3 and 1.0%
*    groups. However, because the incidences for these findings in the control
*    group were comparable, these effects could not be determined to be
*    compound-related. The skeletal abnormalities seen in the sBA groups were
*    consistent in type and frequency with the spontaneous incidence observed
*    in this rat colony.  There were no significant soft tissue findings in
*    the 2% treated group.
F008 CLGETTS
F012 20
F020 120330
EOR
F002 27
F010 5.8.2
F004 2
F005 RS
F006 Maternal NOEL:  1% (1771 mg/kg/day)
**   Maternal NOAEL:  1% (1771 mg/kg/day)
**   Pup NOEL:  1% (1771 mg/kg/day)
F007 Maternal NOEL:  1% (1771 mg/kg/day)
**   Maternal NOAEL:  1% (1771 mg/kg/day)
**   Pup NOEL:  1% (1771 mg/kg/day)
F008 CLGETTS
F012 20
F020 120331
EOB
C
X
```