Via Electronic Submission

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November 14, 2007

Administrator
US Environmental Protection Agency
P. O. Box 1473
Merrifield, VA 22116
Attention: Chemical Right-to-Know Program

Re: C4-6 Isopentene Rich-Ether Fraction (IRF) stream, CAS No. 108083-43-8 for the HPV Challenge Program (ExxonMobil Chemical Company Registration Number for HPV Challenge Program)

To Whom It May Concern:

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. Under the U.S. Environmental Protection Agency (EPA) High Production Volume (HPV) Chemical Challenge Program (Program), ExxonMobil Chemical Company committed to voluntarily compile a Screening Information Data Set (SIDS) that can be used for an initial hazard assessment of the C4-6 Isopentene Rich-Ether Fraction (IRF) stream, CAS No. 108083-43-8. Although there are no data for the stream, based on its composition, it was determined that data for three constituents can be used to characterize the SIDS endpoints because they comprise a large fraction of the stream and therefore, will define the fate and effects of the stream. The three substances are tert-amyl methyl ether (CAS No. 994-05-8), heptane (CAS No. 142-82-5), and cyclohexene (CAS No. 110-83-8).

With this letter, EMCC submits the test plan and robust study summaries compiled into separate dossiers for the three main constituent substances in the C4-6 Isopentene Rich-Ether Fraction (IRF) stream. Sufficient data and information exist to characterize all endpoints in the HPV Program. Therefore, no additional testing is proposed. With the submission of this test plan and dossiers, EMCC has completed its commitment under the HPV Program for the C4-6 Isopentene Rich-Ether Fraction (IRF) stream.

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

Sincerely,

Susan K. Blevins
Global Product Stewardship and Regulatory Affairs Manager
Email: susan.k.blevins@exxonmobil.com

Attachment

Bcc:

EMCC - Houston
R. Brown
C. Fairbrother

EMBSI - Clinton
A. Bachman
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T. Parkerton
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D. Winkelmann

201-16650A

HIGH PRODUCTION VOLUME (HPV)

CHEMICAL CHALLENGE PROGRAM

TEST PLAN For:

C4-6 ISOPENTENE RICH-ETHER FRACTION STREAM

CAS No. 108083-43-8

Prepared by:

ExxonMobil Chemical Company

November 14, 2007

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 a Screening Information Data Set (SIDS) that can be used for an initial hazard assessment of C4-6 Isopentene Rich-Ether Fraction (IRF) stream, CAS No. 108083-43-8.

Existing data and technical analyses adequately characterize the SIDS endpoints for the IRF stream and support a screening-level hazard assessment, which informs the public about the SIDS-based hazards of this substance. Sufficient data and information exist to characterize all endpoints in the HPV Program. Therefore, no additional testing is proposed.

The IRF stream is a complex substance that contains a predominant ether fraction in combination with a larger hydrocarbon fraction. A search for existing studies/information and their review identified adequate data for select constituents to characterize all SIDS endpoints for the stream. Data suggest that the IRF stream generally presents a low order of hazard for human health and low to moderate order of environmental hazard for the predominant groups of constituents as a whole. The predominant constituents of the stream are relatively volatile. Information on their fate in the environment suggests that once in the atmosphere, they will be largely degraded through physical processes at a relatively rapid rate.

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TEST PLAN FOR C4-6 ISOPENTENE RICH-ETHER FRACTION CAS No. 108083-43-8

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 a Screening Information Data Set (SIDS) that can be used for an initial hazard assessment of the C4-6 Isopentene Rich-Ether Fraction (IRF) stream, CAS No. 108083-43-8. Although there are no data for the stream, based on its composition, it was determined that data for three constituents can be used to characterize the SIDS endpoints because they comprise a large fraction of the stream and therefore, will define the fate and effects of the stream. The three substances are tert-amyl methyl ether (CAS No. 994-05-8), heptane (CAS No. 142-82-5), and cyclohexene (CAS No. 110-83-8).

This assessment includes data for selected physicochemical, environmental fate, and mammalian and environmental effect 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 (1999) document titled *Determining the Adequacy of Existing Data*. The following sections describe the IRF stream and its manufacturing process, and data used to characterize the various endpoints in the HPV Program. After a review of the existing data, ExxonMobil Chemical Company believes that data needed to adequately assess all SIDS endpoints have been identified and that additional testing is not necessary.

II. CHEMICAL DESCRIPTION, MANUFACTURING PROCESS, AND USE

The IRF stream is composed of several constituent substances (Table 1). The substances listed in Table 1 are those found at concentrations of greater or equal to 1% in the stream. The predominant chemical fraction in this stream is the methoxypentanes, which can comprise from approximately 43 to 60% of the stream. The major methoxypentane is 2-methoxy-2-methylbutane, which is also referred to as tert-amyl methyl ether (TAME). A second chemical fraction, which can also comprise a large proportion of the stream is the heptanes. This fraction comprises approximately 18 to 24% of the stream. A third fraction, which can also comprise a significant portion of the stream, is cyclohexene, and can be as much as 6 to 9%. Together these three fractions can comprise up to 91% of the stream. All other groups or identified chemicals in Table 1 each comprise less than 5% of the stream.

In the chemical plant, a mostly C5 stream is brought into the isoamylene unit (IAU) from upstream fractionation. To remove the isoamylene (2-methyl-butene-1 and 2-methyl-butene-2), the stream is run across a catalyst that oxygenates the isoamylene into TAME (tertiary-amyl methyl ether) using methanol. This TAME is then fractionated away from the remaining C5 stream, and decomposed back to isoamylene and methanol and recovered as product. In the first methanol reaction, there are side reactions that occur that cause generation of oxygenates heavier than TAME. These

are fractionated off as the IAU heavy co-product (IRF stream). The IRF stream is then used as a feedstock to make hydrocarbon resins.

Table 1. Percent composition ranges of predominant constituents in the C4-6 Isopentene Rich-Ether Fraction stream.

C4-6 ISOPENTENE RICH-ETHER FRACTION STREAM		
Chemical Group/Chemical (~total % composition range)	**Percent Composition Range**	**Constituent***
C5 Oxygenates (~3 - 7)		
	2.5 - 2.9	2-pentanone
	2.8 - 3.9	tert-amyl alcohol
C6 Cyclic Olefin (~6 - 9)		
	5.7 - 8.5	cyclohexene
Methoxypentanes (~43 - 60)		
	2.8 - 3.3	1-methoxy-3-methylbutane
	12.7 - 15.3	2-methoxypentane
	27.7 - 40.9	2-methoxy-2-methylbutane (tert-amyl methyl ether)
Heptanes (~18 - 24)		
	1.6 - 2.4	2,3-dimethylpentane
	2.1 - 3.0	trans-1,3-dimethylcyclopentane
	2.6 - 3.7	cis-1,3-dimethylcyclopentane
	5.2 - 5.6	n-heptane
	6.4 - 9.3	2-methylhexane
Octane (~1 - 2)		
	1.2 - 1.6	2,2,4-trimethylpentane
C10 Olefins (~2)		
	2.1 - 2.3	C10 olefins (unidentified)

* IRF stream constituents at concentration ranges greater than 1%; ranges are based on results from analyses of three different streams.

III. TEST PLAN RATIONALE AND DATA SUMMARY

The predominant constituent chemical groups of the C4-6 Isopentene Rich-Ether Fraction stream include the methoxypentanes (3 constituents) at as much as 60% of the stream, the heptanes (5 constituents) at as much as 24% of the stream, and cyclohexene at as much as 9% of the stream, these combined constituent fractions, which can comprise from 67 to 91% of the stream, will be responsible for the biological effects exhibited by the stream as a whole. The few remaining chemical groups or individual chemical constituents, that are present at levels between 1% to as much as 9%, will not contribute to a greater adverse biological effect than that resulting from the two major groups. Therefore, data from a representative constituent from each of these two groups and cyclohexene will be used to characterize the overall biological and fate characteristics of the stream.

The basic strategy of this test plan for characterizing the human health hazards of the C4-6 Isopentene Rich-Ether Fraction stream is to evaluate data for the major components of the stream. The major chemical components of the stream in the C4-6 Isopentene Rich-Ether Fraction stream have been tested for human health toxicity endpoints. Available data on these components prove to provide sufficient information to develop scientific judgment-based characterizations of the human health effects of the stream for purposes of satisfying HPV program requirements. Therefore, no additional human health toxicity testing is proposed. The hazard characterization for the C4-6 Isopentene Rich-Ether Fraction stream will include the hazards of tert-amyl methyl ether (TAME), n-heptane and cyclohexene.

The environmental fate and effects of the methoxypentanes (ethers) will be characterized by 2-methoxy-2-methylbutane, also referred to as tert-amyl methyl ether (TAME), which has a SIDS dataset. Use of the TAME data to characterize the ether group in this stream is supported by calculated results from the ECOSAR computer model (ECOSAR, 2004) using EPI Suite™ (2000) modeled input data. The 48- or 96-hour data for each of the freshwater fish, daphnid, and green alga endpoints show that the three ethers are expected to cause effects within 20 mg/L of each other. The environmental fate and effects of the heptanes will be characterized by measured and calculated data for n-heptane. The environmental fate and effects of the C6 cyclic olefin component will be characterized by measured and calculated data for cyclohexene.

All TAME test data identified within this document were developed using the parent substance. Additional data for this group used 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 the representative substances.

Data used to characterize the various physicochemical, environmental fate, and environmental and mammalian health endpoints are described below.

A. Physicochemical Data

Calculated and measured TAME, heptane, and cyclohexene physicochemical data from the literature are listed in Table 2.

Table 2. Selected physico-chemical properties for three select constituents used to characterize the C4-6 Isopentene Rich-Ether Fraction stream.

ENDPOINT	TAME*	HEPTANE	CYCLOHEXENE
Melting Point (ºC)	-81.2 (U.S. EPA, 2000)	-90.6 (Lide *et al.*, 1997-1998)	-103.5 (U.S. EPA, 2000)
Boiling Point (ºC at 1012 hPa)	86.3 (Lide *et al.*, 1997-1998)	98.4 (Lide *et al.*, 1997-1998)	82.9 (U.S. EPA, 2000)
Density (g/cm^3 at 20°C)	0.770 (Lide *et al.*, 1997-1998)	0.684 (Lide *et al.*, 1997-1998)	0.81 (Verschueren, 1983)
Vapor Pressure (Pa at 25°C)	12,000 (Huttunen *et al.*, 1997)	6,133 (Daubert & Danner, 1989)	11,865 (Daubert & Danner, 1989)
Water Solubility (mg/l at 25°C)	5,468 (U.S. EPA, 2000)	3.4 (Yalkowsky & Dannenfelser, 1992)	213 (Yalkowsky & Dannenfelser, 1992)
Log K_{ow}	1.55 (20°C) (Huttunen *et al.*, 1997)	4.50 (25°C) (Sangster, 1989)	2.86 (20°C) (Hansch *et al.*, 1995)

* tert-amyl methyl ether

Conclusion

Based on data identified for TAME, n-heptane, and cyclohexene, the IRF stream will exhibit a melting range between approximately -81 to -104°C, a boiling range between approximately 83 to 98°C, a density ranging from approximately 0.8 to 0.7 g/cm^3 at 20°C, and a vapor pressure between approximately 6,133 to 12,000 Pa at 25°C. The predominant constituents of the IRF stream have water solubilities that range from 3.4 to 5,468 mg/l at 25°C and Log K_{ow} values that range from approximately 1.55 to 4.50 (Log K_{ow} values were determined at two different temperatures, 20 and 25°C).

B. 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.

The test guideline used to assess the biodegradability of TAME was OECD 301D, Closed Bottle Biodegradation Test. This test design uses a sealed bottle, which is appropriate considering the test material is relatively volatile. The source of the microbial inoculum used in this study was a domestic wastewater treatment facility and it was not acclimated. TAME exhibited 4% biodegradation after 28 days (Bealing, 1995).

The test guideline used to assess the biodegradability of n-heptane was the standard method for the examination of water and waste water (APHA, 1971). The source of the microbial inoculum used in this study was a silt loam soil and it was not acclimated. The average biodegradation based on theoretical biological oxygen demand for n-heptane on days 2, 5, 10, and 20 was 28, 63, 70, and 70%, respectively (Haines and Alexander, 1974).

Biodegradability of cyclohexene was determined following test guidelines of the Japanese Ministry of International Trade and Industry (MITI). The study design is comparable to OECD 301C (Modified MITI Test). The concentration of cyclohexene in the study was 100 mg/l, with a concentration of 30 mg/l of inoculum. The source of the inoculum was activated sludge and it was not acclimated. Cyclohexene exhibited 0% biodegradation after 28 days, based on BOD (CITI, 1992).

Conclusion

Based on data for TAME and n-heptane, the IRF stream is expected to demonstrate an overall low extent of biodegradation. The ether fraction of the stream, which is the predominant fraction, is not expected to demonstrate significant biodegradation because the constituents that comprise this fraction will biodegrade to a similar extent as was exhibited by TAME. The cyclohexene fraction is also not expected to biodegrade to any appreciable extent. In comparison, the hydrocarbon fraction is expected to demonstrate a higher extent of biodegradability, in particular, the paraffinic fraction as a whole is expected to exhibit a moderate extent of biodegradation with heptane as the potentially most rapidly biodegradable. However, in the environment, the fate of the IRF stream constituents have the potential to partition primarily to air because the they have relatively high vapor pressures, which suggests that they can volatilize to the air at a rapid rate if released.

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). 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,

the ether fraction of the IRF stream is not subject to photolytic processes in the aqueous environment.

Similarly, saturated and unsaturated hydrocarbons like those in the IRF stream do not absorb light above 290 nm. Therefore, the hydrocarbon constituents of this stream will not exhibit photolytic degradation.

Conclusion

Based on the potential for photolysis of ethers and hydrocarbons, this process is not expected to significantly contribute to the degradation of constituents of the IRF stream.

Photodegradation – Atmospheric Oxidation

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

The constituents of the IRF stream have the potential to volatilize to air, based on the vapor pressure of three of the predominant constituents, where they are subject to atmospheric oxidation. In air, IRF stream constituents can react with photosensitized oxygen in the form of hydroxyl radicals ($^{\bullet}OH$). The computer program AOPWIN (atmospheric oxidation program for Microsoft Windows) (U.S. EPA, 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 $^{\bullet}OH$ reaction rate constant and a defined $^{\bullet}OH$ concentration.

TAME has a calculated half-life in air of 24.6 hours or 2.1 days (12-hour day), based on a rate constant of 5.22 x 10^{-12} cm^3/molecule*sec and an $^{\bullet}OH$ concentration of 1.5 x 10^6 $^{\bullet}OH$ /cm^3. Heptane has a calculated half-life in air of 18.7 hours or 1.6 days (12-hour day), based on a rate constant of 6.87 x 10^{-12} cm^3/molecule*sec and an $^{\bullet}OH$ concentration of 1.5 x 10^6 $^{\bullet}OH$ /cm^3. In comparison, cyclohexene has a calculated half-life in air of 2.1 hours or 0.17 days (12-hour day), based on a rate constant of 61.52 x 10^{-12} cm^3/molecule*sec and an $^{\bullet}OH$ concentration of 1.5 x 10^6 $^{\bullet}OH$ /cm^3.

Conclusion

Atmospheric oxidation via hydroxyl radical attack can be a significant route of degradation for constituents in the IRF stream. Based on calculated values for three chemicals that are representative of the majority of stream constituents, IRF stream constituents are expected to have an atmospheric half-life of approximately 2 days or less as a result of indirect photolysis by hydroxyl radical attack.

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 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 (Neely, 1985). The lack of a suitable leaving group renders a compound resistant to hydrolysis. Ether and hydrocarbon constituents of the IRF stream are resistant to hydrolysis because they lack functional groups that are

hydrolytically reactive and Harris (1982b) identifies ether groups as generally resistant to hydrolysis.

Conclusion

Hydrolysis will not contribute to the removal from the environment of constituents in the IRF stream**.**

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 (i.e., air, soil, water, sediment, suspended sediment, and biota). Two widely used fugacity models are the EQC (Equilibrium Criterion) Level I and Level III model (Mackay, 1998a; Mackay, 1998b).

The input data required to run a Level I model include basic physicochemical parameters; distribution is calculated as percent of chemical partitioned to 6 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 to partition, based on 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.

Results of the Mackay Level I and Level III environmental distribution models for three representative stream constituents are shown in Tables 3 and 4, respectively.

Table 3. Environmental distribution as calculated by the Mackay (1998a) Level I fugacity model for select constituents used to characterize the C4-6 Isopentene Rich-Ether Fraction stream.

ENVIRONMENTAL COMPARTMENT	TAME DISTRIBUTION* (%)	HEPTANE DISTRIBUTION** (%)	CYCLOHEXENE DISTRIBUTION† (%)
Air	97.77	99.91	99.82
Water	2.16	<0.01	0.11
Soil	0.07	0.08	0.07
Sediment	<0.01	<0.01	<0.01
Suspended Sediment	<0.01	<0.01	<0.01
Biota	<0.01	<0.01	<0.01

* Distribution is based on the following model input parameters for TAME (tert-amyl methyl ether):

Molecular Weight	102.18
Temperature	25° C
Log K_{ow}	1.55
Water Solubility	5,468 g/m^3
Vapor Pressure	12,000 Pa
Melting Point	-81.22° C

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

Molecular Weight	100.21
Temperature	25° C
Log K_{ow}	4.50
Water Solubility	3.4 g/m^3
Vapor Pressure	6,133 Pa
Melting Point	-90.6° C

† Distribution is based on the following model input parameters for cyclohexene:

Molecular Weight	82.15
Temperature	25° C
Log K_{ow}	2.86
Water Solubility	213 g/m^3
Vapor Pressure	11,865 Pa
Melting Point	-103.5° C

Table 4. Environmental distribution as calculated by the Mackay (1998b) Level III fugacity model for select constituents used to characterize the C4-6 Isopentene Rich-Ether Fraction stream.

ENVIRONMENTAL COMPARTMENT	TAME DISTRIBUTION* (%)	HEPTANE DISTRIBUTION** (%)	CYCLOHEXENE DISTRIBUTION† (%)
Air	26.2	26.0	3.0
Water	55.2	48.5	78.5
Soil	18.6	13.9	17.3
Sediment	0.1	11.6	1.2

* Distribution for TAME (tert-amyl methyl ether) is based on the following model input parameters, reaction half-life in hours as predicted using EPI SuiteTM (2000), and a model default emission rate of 1000 kg/hr into each of the air, water, and soil compartments:

Molecular Weight	102.18	Reaction half-life (hr):	
Temperature	25° C	Air (gaseous)	46.7
Log K_{ow}	1.55	Water (no susp. part.)	360
Water Solubility	5,468 g/m^3	Bulk Soil	720
Vapor Pressure	12,000 Pa	Bulk Sediment	3,240
Melting Point	-81.22° C		

** Distribution for heptane is based on the following model input parameters, reaction half-life in hours as predicted using EPI SuiteTM (2000), and a model default emission rate of 1000 kg/hr into each of the air, water, and soil compartments:

Molecular Weight	100.21	Reaction half-life (hr):	
Temperature	25° C	Air (gaseous)	35.9
Log K_{ow}	4.50	Water (no susp. part.)	208
Water Solubility	3.4 g/m^3	Bulk Soil	416
Vapor Pressure	6,133 Pa	Bulk Sediment	1,870
Melting Point	-90.6° C		

† Distribution for cyclohexene is based on the following model input parameters, reaction half-life in hours as predicted using EPI SuiteTM (2000), and a model default emission rate of 1000 kg/hr into each of the air, water, and soil compartments:

Molecular Weight	82.15	Reaction half-life (hr):	

Temperature	25° C	Air (gaseous)	2.09
Log K_{ow}	2.86	Water (no susp. part.)	360
Water Solubility	213 g/m^3	Bulk Soil	720
Vapor Pressure	11,865 Pa	Bulk Sediment	7,200
Melting Point	-103.5° C		

Conclusion

Results of the Mackay Level I model suggest that the predominant constituents of the IRF stream will partition primarily to the air, >97%. These results are largely explained by their vapor pressures. In comparison, the Level III model suggests that the majority of the IRF stream will partition to the water compartment, approximately 49 to 78%, followed by the air compartment at approximately 3 to 26%, and soil compartment at approximately 14 to 19%. These results are explained by the model parameters, but in particular the default emission rates and degradation half-lives.

C. Aquatic Toxicity Data

Data are available to characterize the potential freshwater fish acute, invertebrate acute, and freshwater alga toxicity of the IRF stream, based on data for three constituents, TAME, n-heptane, and cyclohexene (Tables 5 through 7). TAME demonstrated a measured 96-hour trout (*Oncorhynchus mykiss*) LC_{50} toxicity value of 580 mg/L (API, 1995a) and a measured 48-hour invertebrate (*Daphnia magna*) EC_{50} toxicity value of 100 mg/L (API, 1994). The lowest green alga (*Selenastrum capricornutum*) 72-hour EC_{50} toxicity value was for biomass and measured 230 mg/L (Fortum, 2003). The 72-hour NOEC value from this study was 77 mg/L.

The measured TAME data were compared with data calculated (Table 5) by the ECOSAR model (2004). This model is considered appropriate to estimate the aquatic toxicity for this class of chemicals. The calculated data compared favorably with the measured data. The calculated freshwater fish acute, invertebrate acute, and freshwater alga toxicity values ranged between 127 to 208 mg/L.

Table 5. Measured and calculated aquatic toxicity values for TAME (tert-amyl methyl ether).

ENDPOINT	MEASURED VALUE (mg/L)	CALCULATED VALUE* (mg/L)
Fish 96-hr LC_{50}	580 (API, 1995a)	201
Daphnid 48-hr EC_{50}	100 (API, 1994)	208
Alga 72-hr EbC_{50}	230 (Fortum, 2003)	na
Alga 96-hr EC_{50}	na	127
Alga 72-hr NOEC	77 (Fortum, 2003)	na
Alga 96-hr ChV**	na	10**

na - not available

* Model input parameters for ECOSAR (2004):

Log K_{ow}	1.55
Water Solubility	5,468 g/m^3
Melting Point	-81.2° C

** ChV (chronic) value

Measured n-heptane data are available for a freshwater invertebrate and two marine invertebrate species (Table 6). Heptane demonstrated a 48-hour invertebrate (*Daphnia magna*) EC_{50} toxicity value of 1.5 mg/L (TNO, 1986). Two marine invertebrate species, *Chaetogammarus marinus* and *Mysidopsis bahia*, demonstrated 96-hour LC_{50} toxicity values of 0.2 and 0.1 mg/L, respectively (TNO, 1986).

The measured n-heptane data were compared with data calculated (Table 6) by the ECOSAR model (2004). This model is considered appropriate to estimate the aquatic toxicity for this class of chemicals. The calculated data compared favorably with the measured data. The calculated freshwater fish acute, invertebrate acute, and freshwater alga toxicity values ranged between 0.3 to 0.4 mg/L.

Table 6. Measured and calculated aquatic toxicity values for n-heptane.

ENDPOINT	MEASURED VALUE (mg/L)	CALCULATED VALUE* (mg/L)
Fish 96-hr LC_{50}	na	0.33
Daphnid 48-hr LC_{50}	1.5 (TNO, 1986)	0.42
Alga 96-hr EC_{50}	na	0.31
Alga 96-hr ChV**	na	0.13
Marine Invert. 96-hr LC_{50}	0.2 (TNO, 1986)	na
Marine Invert. 96-hr LC_{50}	0.1 (TNO, 1986)	na

na - not available

* Model input parameters for ECOSAR (2004):
Log K_{ow} 4.50
Water Solubility 3.4 g/m^3
Melting Point -90.6° C

** ChV - chronic value

Measured cyclohexene data are available for a freshwater fish (Table 7). Cyclohexene demonstrated a 96-hour medaka (*Oryzias latipes*) LC_{50} toxicity value of >10 mg/L (CITI, 1992). An additional study with Coho Salmon (*Oncorhynchus kisutch*) reported no significant mortalities up to 100 ppm (Morrow *et al.*, 1975) for cyclohexene in artificial seawater. However, the study was performed in open vessels, and therefore the data was considered questionable.

The measured cyclohexene data were compared with data calculated (Table 7) by the ECOSAR model (2004). This model is considered appropriate to estimate the aquatic toxicity for this class of chemicals. The calculated data compared favorably with the measured data. The calculated freshwater fish acute, invertebrate acute, and freshwater alga toxicity values ranged between 5.8 to 8.7 mg/L.

Table 7. Measured and calculated aquatic toxicity values for cyclohexene.

ENDPOINT	MEASURED VALUE (mg/L)	CALCULATED VALUE* (mg/L)
Fish 96-hr LC_{50}	>10	7.6
Daphnid 48-hr LC_{50}	na	8.7
Alga 96-hr EC_{50}	na	5.8
Alga 96-hr ChV**	na	1.0

na - not available

* Model input parameters for ECOSAR (2004):
Log K_{ow} 2.86
Water Solubility 213 g/m^3
Melting Point -103.5° C

** ChV - chronic value

Conclusion

The predominant constituent chemical groups of the C4-6 Isopentene Rich-Ether Fraction stream include the methoxypentanes (3 constituents), which when combined can range from approximately 43 to 60% of the stream, the heptanes (5 constituents), which when combined can range from approximately 18 to 24% of the stream, and cyclohexene, which can range from 6 to 9% of the stream. These combined constituent fractions, which can comprise up to 91% of the stream, will be responsible for the biological effects exhibited by the stream as a whole. Although the methoxypentanes (represented by toxicity data for TAME) comprise the larger percentage of the stream, they demonstrate much lower toxicity in comparison to the heptanes (represented by toxicity data for n-heptane). Cyclohexene also demonstrates much lower toxicity in comparison to n-heptane. The heptanes are contained by the IRF stream in sufficient concentration to exert effects on fish, invertebrates, and algae at levels demonstrated by n-heptane. Therefore, the effect range characterized by the data for n-heptane represents the potential aquatic toxicity of the IRF stream, which can range from 0.1 to 1.5 mg/L.

D. Mammalian Toxicity Data

Acute Toxicity

Data are available to characterize the potential acute toxicity of the C4-6 Isopentene Rich-Ether Fraction stream, based on data for three constituents, Tertiary amyl methyl ether (TAME), cyclohexene and n-heptane. The oral rat LD_{50} values for TAME and cyclohexene were approximately 2100 mg/kg (Daughtrey and Bird, 1995) and 1000-2000 mg/kg (OECD, 2002), respectively. The dermal LD_{50} values for TAME and cyclohexene were >3160 mg/kg (ExxonMobil, 1985a) and >20 mL/kg (OECD, 2002), respectively. The inhalation rat LC_{50} values for TAME and n-heptane were >5.4 mg/L (Amoco, 1991a) and >29 mg/L (HEDSET, 1982), respectively. Four-hour inhalation exposure of rats to 21388 mg/m^3 (6370 ppm) cyclohexene produced no deaths (OECD, 2002).

In summary, available acute toxicity data on predominant constituents of the C4-6 Isopentene Rich-Ether Fraction stream demonstrated a low order of acute oral, dermal, and inhalation toxicity. No further testing is proposed.

Genotoxicity

In vitro

Three constituents of the C4-6 Isopentene Rich-Ether Fraction stream have been evaluated in several *in vitro* genotoxicity assays. TAME, cyclohexene and n-heptane were negative in a bacterial reverse gene mutation assay (Ames test) in *Salmonella typhimurium* and/or *Escherichia coli* with and without S-9 metabolic activation (Brooks et al., 1982; Daughtrey and Bird, 1995; OECD, 2002). Cyclohexene and n-heptane showed no evidence of genotoxic activity in the mammalian chromosomal aberration assays (Brooks et al., 1982; OECD, 2002). n-Heptane was also negative in a mitotic gene conversion assay using *Saccharomyces cerevisiae* JD1 (Brooks et al., 1982).

TAME was tested in an *in vitro* Mammalian Chromosomal Aberration Test (American Petroleum Institute, 1997b). In this study, TAME was tested in cultured Chinese hamster ovary (CHO) cells for induction of chromosomal aberrations, both in the presence and absence of Aroclor 1254-induced Sprague-Dawley rat liver S9. The test included concurrent solvent and positive controls and five doses of TAME. The doses tested were 313, 625, 1250, 2500, and 5000 μg/ml. In the absence of S9, a statistically significant increase in aberrant cells was observed at 2500 and 5000 ug/ml, and a dose response was observed. In the presence of S9, a statistically significant increase in aberrant cells was observed at all concentrations, and a dose response was observed. In conclusion, based on these results, TAME was clastogenic under the conditions of this assay.

In vivo

TAME was evaluated *in vivo* for its ability to induce micronuclei in bone marrow polychromatic erythrocytes (PCEs) in CD-1 mice (Daughtrey and Bird, 1995). TAME was diluted in corn oil and administered as a single intraperitoneal injection at doses of 0.15, 0.375, and 0.75 g/kg. Cyclophosphamide was dissolved in water and used as the positive control at a dose of 40 mg/kg. Animals from the appropriate groups were euthanized by CO_2 at approximately 24, 48 and 72 hours after administration of test article. Animals dosed with cyclophosphamide were taken at 24 hours only. Each group consisted of 10 animals (5/sex/group) per time point. At death, both femurs from each animal were removed and bone marrow was recovered and suspended in fetal bovine serum. Bone marrow slides were prepared and stained with acridine orange prior to microscopic evaluation. One thousand polychromatic erythrocytes from each animal were examined for micronuclei formation. In addition, the ratio of polychromatic erythrocytes (PCEs) to normochromatic erythrocytes (NCEs) was determined by counting 1000 erythrocytes (PCEs and NCEs). No increase in micrucucleus frequency was observed at any dose level of TAME or at any of the bone marrow collection times. The positive control produced statistically significant increases in micronucleus frequencies in both males and females. Overt marrow toxicity, as measured by a statistically significant decrease in the percentage of polychromatic erythrocytes, was not observed in any of the groups dosed with TAME. The percentages of polychromatic erythrocytes observed were within the normal range. Thus, these data indicated that

TAME did not cause clastogenic effects in mouse bone marrow.

In summary, *in vitro* genotoxicity testing of cyclohexene and n-heptane demonstrated no evidence of genotoxicity. TAME was not mutagenic in an *in vitro* Ames assay but was found to be clastogenic in an *in vitro* chromosome aberration study. However, as no evidence of genotoxicity was observed in an *in vivo* mouse micronucleus test, the weight of evidence suggests that TAME is not a mutagen. Based on these data on predominant constituents, no additional testing on the C4-6 Isopentene Rich-Ether Fraction stream is proposed.

Repeated Dose Toxicity

A number of repeated dose toxicity studies have been conducted on TAME, cyclohexene and n-heptane.

A 28-day repeated dose inhalation toxicity study was conducted with TAME vapor in Sprague-Dawley rats (Amoco, 1991a; White *et al.*, 1995). In this study, the rats (14/sex/group) were exposed to TAME vapor at target concentrations of 0, 500, 2000, and 4000 ppm for 6 hours per day, 5 days per week for 4 weeks. Three out of 14 males and 4 out of 14 females in the 4000 ppm group died during the study, three animals during the first week, two during the second week and two during the third week. The 2000 ppm and 4000 ppm groups showed signs of central nervous system depression as well as other signs of toxicity, e.g., lacrimation, dyspnea, rales, diarrhea, piloerection, etc. Significant decreases in body weight gain were observed in the 4000 ppm males resulting in significantly reduced mean body weights during weeks 2 - 4. No other significant effects on body weight were reported. Evaluation of gross pathology revealed that absolute brain weights were significantly decreased in the 4000 ppm males and that absolute liver weights were significantly increased in the 2000 ppm males and 4000 ppm females. Many relative organ weights were increased for the 4000 ppm males due to the reduced body weights of these animals. No treatment-related histopathological findings were noted. TAME produced minimal effects on clinical chemistry and hematology parameters. A No Observed Adverse Effect Level (NOAEL) of 500 ppm was determined in this study.

A 28-day repeated oral dose toxicity study was conducted with TAME in Sprague-Dawley rats (Daughtrey and Bird, 1995). In this study, the rats (5/sex/group) were dosed with 0, 125, 500, and 1000 mg/kg TAME in corn oil by gavage at a dose volume of 2 ml/kg. Vehicle control animals received corn oil only. The dosing regimen was once daily, 7 days a week, for a period of 29 days.

Four animals (two male, two female) in the high-dose group died during the course of the study. Of these four, two deaths were attributed to dosing accidents. The remaining two deaths were presumed to be test material-related, although a precise cause of death could not be identified. All other animals survived to the scheduled termination. Overall, in-life observations were unremarkable. Lung rales and anogenital staining of the fur were observed at a low frequency in the high-dose group. The majority of animals of either sex did not exhibit any unusual symptoms or behaviors. Mean body weights of high-dose males were significantly lower than those of control males at day 7, day 21, and day 28. Mean body weight gain in high-dose females was also lower than in control females, although the difference was not statistically significant. Food consumption in high-dose males and females was also

significantly reduced compared to controls during week 1. During week 2, food consumption was significantly reduced only in high dose males. A dose-related increase in adrenal weights was observed that was statistically significant in the mid- and high-dose males. A similar increase in adrenal weights was not observed in female rats dosed with TAME. Relative kidney weights were also increased in mid- and high-dose male rats compared to control.

Hematology and serum chemistry values were generally similar across dose groups. Activated partial thromboplastin time was statistically increased in the high-dose male (but not female) group. However, this small increase was not believed to be biologically meaningful. The mean serum glucose value was also significantly reduced in the high-dose male group. The biological significance of this finding was unknown, however a similar decrease in serum glucose was not observed in high-dose females. No treatment-related tissue lesions were observed during the histopathological examination. Any changes observed were limited to naturally occurring lesions that were present in approximately equal frequency in all groups, including controls. Of note, the organ weight increases observed in the kidney and adrenals were not accompanied by any histopathological changes. The NOAEL in this study was determined to be 500 mg/kg/day.

In a 13-week repeated dose toxicity study conducted by the American Petroleum Institute (1997a), F344 rats (51/sex - control and high dose; 41/sex - low and mid-dose) and CD-1 mice (46/sex -control and high dose; two groups each; 36/sex -low and mid-dose) were exposed by whole body inhalation to TAME at target concentrations of 0, 240, 1500, and 3500 ppm for 6 hours/day, 5 day/week for 13 weeks (minimum 65 exposures). A new high dose group of mice at 2500 ppm and corresponding control group were established due to high mortality at 3500 ppm. The results for rats and mice are presented separately.

In rats, a number of effects were observed at the highest dose used, 3500 ppm. These effects included a low incidence of mortality (2/102), abnormal clinical signs (lethargy and prostration), acute neurological effects, decreased body weight and body weight gain, effects on hematology (increased platelet counts), effects on clinical chemistry (increases in total protein, albumin and globulin), and a number of effects on organ weights. The effects on the kidneys of the male rats were consistent with the male rat specific α2u-globulin syndrome and were not considered to be relevant to risk assessment in humans. Exposure of rats at 1500 ppm resulted in effects including post exposure clinical signs, acute neurological effects (males only), increased platelet count in males, increases in total protein, albumin and globulin and effects on liver and kidney (only in females) weight. An increase in liver weights of male rats exposed to 250 ppm was also observed. Many of these resolved after the 4 week recovery period. On histopathological examinations, no dose-related changes were observed in the liver. No test material-related changes in motor activity were observed at any doses. The NOAEL for rats was 1500 ppm in this study.

In this study, high mortality was observed in mice exposed to 3500 and 3000 ppm. A number of effects were observed at the highest dose used in the main study, 2500 ppm. These included 27 deaths among 92 mice, post-exposure clinical signs, effects on a number of clinical chemistry parameters, and increased liver weights. Exposure of mice at 1500 ppm resulted in effects including post exposure clinical signs, increased globulin

in males at week 6 and effects on liver weights in males. Many of these resolved after the 4 week recovery period. Liver cell proliferation studies showed increases in the labelling index of hepatocytes and centrilobular hepatocellular hypertrophy was observed in the 2500, 1500 and 250 ppm animals. Centrilobular hepatocellular hypertrophy is considered an adaptive response to increased metabolic load. The NOAEL for mice was determined to be 1500 ppm.

Effects of repeated exposure to cyclohexene were evaluated as part of an OECD 422, combined repeated toxicity study with reproductive/developmental toxicity screen in SD rats (OECD, 2002). Twelve male and twelve female rats received gavage doses of 0 (corn oil), 50, 150 and 500 mg/kg/day cyclohexene. Males were dosed for 48 days and females for 42-53 days from 14 days before mating to day 4 of lactation throughout the mating and pregnancy period. Salivation was observed in 3 of 12 males and 2 of 12 females at 150 mg/kg/day and in all of 12 males and 12 females at 500 mg/kg/day. This sign was observed only for about 5 minutes after dosing at 150 mg/kg/day but up to 6 hours after dosing at 500 mg/kg/day. No significant changes of body weight, food consumption and hematological findings for both sexes and urinalysis findings for males were detected. Blood chemical examination showed a decrease in triglyceride in males at 150 and 500 mg/kg/day, and increases in total bilirubin in males at 500 mg/kg/day and in total bile acid in females at 50 mg/kg/day and in both sexes at 150 mg/kg/day and above. In males of the 500 mg/kg/day group, there was an increase in relative kidney weight. On histopathological examinations, no dose-related changes were observed. The increase in total bile acid observed in females at 50 mg/kg/day was not considered to be an adverse effect because of no accompanying changes. Therefore, based on salivation at 150 mg/kg/day and above, the NOAEL for repeated dose toxicity was considered to be 50 mg/kg/day for both sexes.

A 26-week inhalation toxicity study with n-heptane was conducted in Sprague-Dawley rats (API, 1980). In this study, the rats (15/sex/group) were exposed by inhalation to 0, 398 and 2970 ppm n-heptane for 6 hours/day, 5 day/week for 26 weeks. There were no treatment-related deaths during the study. The only treatment-related observations were labored breathing or rapid breathing and slight prostration during the first week of study during exposure only, and anogenital fur staining and dry rales during weekly observations. No significant changes of body weight, hematology or urinalysis for both sexes were detected. Serum alkaline phosphatase was significantly elevated in female high dose rats and slightly elevated in low dose females. All other clinical chemistry values appeared normal with the exception of one male in the high dose group whose serum glutamic pyruvic transaminase and serum alkaline phosphatase levels were markedly elevated when compared to all other male rats on test. Proteinuria, elevated specific gravity and ketones were observed but do not appear to be related to treatment. The effects observed are consistent with acute central nervous system (CNS) depression and generally abated by the second week of the study. Under the conditions of this study, the Low Observed Adverse Effect Level (LOAEL) for acute CNS depression was 2970 ppm and the NOAEL for systemic toxicity was 2970 ppm.

In a 30-week inhalation neurotoxicity study, Sprague-Dawley rats (6-9 males/dose group) were exposed by inhalation to air or 1500 ppm n-heptane for 9 hours/day, 5 days/week for 30 weeks (Frontali et al., 1981). The primary objective of this study was to assess the appearance of polyneuropathy and urinary metabolites in rats following exposure to analytical grade solvents frequently used in Italian shoe factories. Nerve

tissue was examined microscopically. None of the animals developed signs of neuropathy. There were no differences in weight gain of rats exposed to n-heptane compared to controls. Differences between mean values for hindlimb spreads observed in treated animals and controls were not statistically significant. No histological signs of giant oxonal degeneration were noted in rats treated at 1500 ppm. Under the condition of this test, the NOAEL for repeated dose toxicity was considered to be 1500 ppm.

In summary, data are available to adequately characterize the repeated dose toxicity of C4-6 Isopentene Rich-Ether Fraction (IRF) stream. The IRF stream is expected to have a low order of repeated dose toxicity. No further testing is proposed.

Reproductive and Developmental Toxicity

Predominant constituents of the C4-6 Isopentene Rich-Ether Fraction stream have been evaluated for reproductive and developmental toxicity.

A two-generation reproductive toxicity study of inhaled TAME vapor was conducted in Sprague-Dawley rats (Tyl *et al.*, 2003). In this study, weanling F0 rats (30/sex/group) inhaled TAME vapor at 0, 250, 1500, or 3000 ppm 5 day/week and 6 h/day for 10 weeks, with vaginal cytology evaluated for weeks 8-10. The F0 animals then produced F1 offspring, with exposure 7 days a week from mating through to lactation. During the F1 prebreed exposure period, vaginal patency, preputial separation (PPS) and vaginal cytology were evaluated. The F1 animals were mated, with F2 anogenital distance measured on postnatal day zero. At F2 weaning 30 of each gender per group were selected for postwean retention, with no exposures, through vaginal patency and PPS. Body weights, feed consumption and clinical signs were recorded throughout the study. Adult F0 and F1 systemic toxicity was present at 1500 and 3000 ppm. Minor adult male reproductive toxicity was present at 3000 ppm. There were no adult effects on vaginal cyclicity, estrous cycle length, mating, fertility, pregnancy, gestational length or ovarian and uterine weights. There were no treatment-related gross or histopathologic findings in parental male or female systemic or reproductive organs. Offspring toxicity was present at 1500 and 3000 ppm. The NOAEL for adult reproductive toxicity was 1500 ppm for males and 3000 ppm for females. The NOAEL for offspring toxicity was 250 ppm in rats under the conditions of this study.

A developmental toxicity study was conducted by TAME vapor inhalation exposure in two pregnant rodent species (Welsch *et al.*, 2003). Timed-pregnant Sprague-Dawley rats and CD-1 mice, 25 animals per group, inhaled TAME vapors containing 0, 250, 1500, or 3500 ppm for 6 hours a day on gestational days (gd) 6-16 (mice) or 6-19 (rats). The developmental toxicity hazard potential was evaluated following the study design draft guidelines and end points proposed by the United States Environmental Protection Agency.

In the present study, inhalation of TAME by pregnant rats from gestational days 6-19 resulted in manifestations of maternal toxicity at 1500 and 3500 ppm. These effects were expressed by reductions in body weight (at 3500 ppm only), feed consumption and weight gain, and TAME exposure-induced clinical signs of toxicity. There was no evidence of maternal toxicity at 250 ppm. The increased maternal relative liver weight at 3500 ppm that occurred when maternal body weight was actually reduced may be due to induction of metabolizing enzymes and a concurrent increase in liver mass. There was a clear indication of maternal accommodation to the highest TAME exposure

concentration, as evidenced by diminution in incidence and intensity of clinical signs such as ataxia, lethargy and slow respiration over time. Developmental toxicity occurred only at 3500 ppm and was expressed as reduced fetal body weights per litter. There was no evidence of treatment-related teratogenicity at any of the three exposure concentrations and no other developmental effects. Almost all of the fetal malformation and variation findings were those commonly observed in historical control Sprague-Dawley rat fetuses and in published control databases. Therefore, the NOAEL was 250 ppm for maternal toxicity and 1500 ppm for developmental toxicity in rats under the conditions of this study.

In mice, the inhalation of TAME vapors during gd 6-16 resulted in maternal toxicity at 3500 ppm, including maternal mortality (4/25), reductions in body weight, weight gain and treatment-related clinical signs of toxicity. At 1500 ppm, mice exhibited reduced feed consumption (only for gd 6-9) and limited treatment-related clinical signs of toxicity. There was no evidence for maternal toxicity at 250 ppm. The increased maternal absolute and relative liver weights at 1500 and 3500 ppm may have been due to induction of metabolizing enzymes and therefore increase in tissue mass. There was also a clear indication of reduced pharmacological effects with time and maternal accommodation to the top two exposure concentrations. This interpretation was supported by observations of mortality at 3500 ppm early in the exposure period (gd 6-9) only and diminution over time in the incidence of clinical signs of toxicity, such as ataxia, lethargy, gasping and slow respiration. The increased relative liver weight may have been due, at least in part, to the reduced body weights of the dams at termination at 3500 ppm. Developmental toxicity was present at 3500 ppm, expressed specifically as increased incidence of late fetal deaths, reduced fetal body weights per litter and increased incidences of cleft palate (an external malformation) and of enlarged lateral ventricles of the cerebrum (a visceral variation). At 1500 ppm, three fetuses in three litters also exhibited cleft palate (with none observed at 250 or 0 ppm). This increase was not statistically significant, but it is considered biologically relevant and related to maternal TAME exposure. The finding of one additional litter at 1500 ppm with three multiply malformed fetuses (out of nine live fetuses total) may be unrelated to treatment because these malformations were not observed at 3500 ppm and were limited to only one litter at 1500 ppm. The observation of cleft palate in fetuses at 1500 and 3500 ppm appears to be consistent with a proposed mechanism for cleft palate in mice exposed to methyl tertiary butyl ether (MTBE). Maternal exposure to MTBE with anesthetic qualities at high concentrations associated with maternal stress results in elevated endogenous corticosteroid levels, which cause cleft palate to the developing offspring in mice (Bevan *et al.*, 1997). Although those hormone levels were not determined in the present study, the biological mode of action of TAME appears to be similar and comparable to that of MTBE, as judged by clinical observations. At high exposure concentrations in mice, TAME exerts depressant effects on the central nervous system that resemble anesthetic properties and are preceded by a pronounced excitatory stage. Therefore, the brain stimulation and excitation may have induced a rise in endogenous corticosteroid levels in the mouse dams. The occurrence of a significantly increased incidence of fetal cleft palate at the 3500 ppm exposure level, coincident with maternal toxicity, suggests that stress of the dams is a contributing factor. Mice are sensitive to stress, and cleft palate occurs in offspring if the pregnant dams experience stress such as food and water deprivation, transportation, restraint or low humidity. That corticosteroids cause cleft palate in susceptible mouse strains is well documented.

The increased incidence of enlarged lateral ventricles of the fetal cerebrum at 3500 ppm is consistent with developmental delay because the fetuses at this exposure concentration exhibited mean body weights per litter of about 60% of the concurrent control group values. There were no notable developmental effects at 250 ppm. Therefore, the NOAEL for maternal and developmental toxicity in mice was 250 ppm in the present study.

In an OECD 422, combined repeated toxicity study with reproductive/developmental toxicity screen, cyclohexene was administered to SD(Crj:CD)IGS rats by gavage at doses of 0, 50, 150 and 500 mg/kg/day for 48 days from 14 days prior to mating in males and for 42-53 days from 14 days prior to mating to day 4 of lactation throughout the mating and pregnancy period in females (OECD, 2002). Regarding the reproductive ability of parent animals, no effects were detected on the estrus cycle, copulation index, fertility index, gestation length, numbers of corpora lutea and implantations, implantation index, gestation index, delivery index, parturition or maternal behavior. Regarding the developmental parameters, no effects were detected on viability, body weight, general appearance or autopsy findings of offspring. The NOAEL for reproduction/developmental toxicity was considered to be 500 mg/kg/day.

The available data on predominant constituents of the C4-6 Isopentene Rich-Ether Fraction (IRF) stream prove adequate to support a screening level assessment of the reproductive and developmental toxicity of the IRF stream. Furthermore, these data indicate that the IRF stream is expected to have a low order of reproductive and developmental toxicity.

Conclusion

Mammalian toxicology data on three constituents of the IRF stream, TAME, n-heptane and cyclohexene, have shown a low order of acute toxicity by the oral, dermal and inhalation routes of exposure. Repeated exposure to these constituents is not expected to produce target organ toxicity nor cause harm to reproduction or the developing fetus. There is no evidence of causing adverse effects on genetic material. The available data compiled for predominant constituents prove adequate to support a screening level hazard assessment of the IRF stream. Therefore, no additional human health toxicity testing is proposed.

Table 8. Mammalian toxicity endpoint summary for TAME.

TOXICITY ENDPOINT		RESULTS	REFERENCE
Acute	Inhalation	LC50 >5.4 mg/L	Amoco, 1991a
	Oral	LD50 = ~2100 mg/kg	Daughtrey and Bird, 1995
	Dermal	LD50 >3160 mg/kg	ExxonMobil, 1985a
Irritation	Skin	Minimal irritant	Amoco, 1991b
	Eye	Minimal irritant	ExxonMobil, 1985b
Sensitization		Not a dermal sensitizer	American Petroleum Institute, 1995b
Repeated Dose		Rat: NOAEL = 1500 ppm Mouse: NOAEL = 1500 ppm	American Petroleum Institute, 1997a
Reproductive		NOAEL for adult reproductive toxicity = 1500 ppm (males), >3000 ppm (females) NOAEL for offspring toxicity = 250 ppm	Tyl *et al.*, 2003
Developmental		NOAEL for maternal toxicity = 250 ppm (rat, mouse) NOAEL developmental toxicity = 1500 ppm (rat), 250 ppm (mouse)	Welsch, 2003
Neurotoxicity		Acute CNS depression were only observed at high doses immediately after exposure. All effects were completely reversible within 24 hours.	American Petroleum Institute, 1997a
Genotoxicity	*In vitro* Ames *Salmonella* assay	Negative	Daughtrey and Bird, 1995
	In vitro chromosome aberration	Positive - TAME was clastogenic under the conditions of this assay	American Petroleum Institute, 1997b
	In vivo micronucleus	Negative - TAME was not clastogenic to mouse bone marrow	Daughtrey and Bird, 1995

Table 9. Mammalian toxicity endpoint summary for Cyclohexene.

TOXICITY ENDPOINT		RESULTS	REFERENCE
Acute	Inhalation	LC50 >21388 mg/m^3	OECD, 2002
	Oral	LD50 = 1000-2000 mg/kg	
	Dermal	LD50 >16220 mg/kg	
Irritation	Skin		
	Eye		
Sensitization			
Repeated Dose		NOAEL = 50 mg/kg/day (rat)	
Reproductive		NOAEL = 500 mg/kg/day (rat)	
Developmental		NOAEL = 500 mg/kg/day (rat)	
Neurotoxicity			
Genotoxicity	*In vitro* Ames *Salmonella* assay	Negative	
	In vitro chromosome aberration	Negative	
	In vivo micronucleus		

Table 10. Mammalian toxicity endpoint summary for n-Heptane.

TOXICITY ENDPOINT		RESULTS	REFERENCE
Acute	Inhalation	LC50 >29.29 mg/L	HEDSET, 1982
	Oral		
	Dermal		
Irritation	Skin		
	Eye		
Sensitization			
Repeated Dose		NOAEL = 2970 ppm (rat)	American Petroleum Institute, 1980
Reproductive			
Developmental			
Neurotoxicity		No signs of neuropathy and no histological evidence of giant axonal degeneration were noted in rats.	Frontali et al., 1981
Genotoxicity	*In vitro* Ames *Salmonella* assay	Negative	Brooks et al., 1982
	In vitro chromosome aberration	Negative	Brooks et al., 1982
	In vivo micronucleus		

IV. TEST PLAN SUMMARY

A search for existing studies/information identified adequate data to characterize all endpoints under the U.S. EPA HPV Program using data from representative constituents of the predominant fractions in the IRF stream. The three constituents were TAME, n-heptane and cyclohexene. Adequate data for TAME, n-heptane and cyclohexene are shown in Table 11.

Table 11. TAME, cyclohexene, and n-heptane data availability and adequacy for endpoints in the HPV Program.

	Mammalian Toxicity						**Environmental Toxicity**			**Environmental Fate**				**Physical/Chemical Properties**					
	Acute Tox.	Genetic Pt. Mut.	Genetic Chrom.	Repeat Dose	Devel.	Repro.	Acute Fish	Acute Invert.	Alga Tox.	Photo-deg.	Hydrol.	Fug.	Biodeg.	Melt. Pt.	Boil. Pt.	Dens.	Vap. Pres.	Water Sol.	K_{ow}
TAME	**A**	**A**	**A**	**A**	**A**	**A**	**A/C**	**A/C**	**C**	**T**	**T**	**C**	**A**	**A**	**A**	**A**	**A**	**A**	**A**
Cyclohexene	**A**	**A**	**A**	**A**	**A**	**A**	**C**	**C**	**A/C**	**T**	**T**	**C**	**-**	**A**	**A**	**A**	**A**	**A**	**A**
Hep-tane	**A**	**A**	**A**	**A**	**-**	**-**	**C**	**A/C**	**C**	**T**	**T**	**C**	**A**	**A**	**A**	**A**	**A**	**A**	**A**

A Adequate measured data available
C Adequate computer model data available
T Adequate technical discussion available

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I U C L I D

Data Set

Existing Chemical	:	ID: 110-83-8
CAS No.	:	110-83-8
EINECS Name	:	Cyclohexene
EC No.	:	203-807-8
TSCA Name	:	Cyclohexene
Molecular Formula	:	C6H10
IUPAC Name	:	Cyclohexene

Producer related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	06.10.2006

Substance related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	06.10.2006
Status	:	
Memo	:	U.S. EPA - HPV Challenge Program
Printing date	:	01.10.2007
Revision date	:	
Date of last update	:	10.07.2007
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

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	**:**	

18.04.2007

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

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	:	= -103.5 °C
Sublimation	:	
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	
Test substance	:	CAS No. 110-83-8; cyclohexene; purity is unknown
Reliability	:	(2) valid with restrictions 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

18.04.2007 (16)

2.2 BOILING POINT

Value	:	= 82.9 °C at 1013 hPa
Decomposition	:	
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	
Test substance	:	CAS No. 110-83-8; cyclohexene; purity is unknown
Reliability	:	(2) valid with restrictions 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

18.04.2007 (16)

2.3 DENSITY

Type	:	density
Value	:	= .81 g/cm³ at 20 °C
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	
Test substance	:	CAS No. 110-83-8; cyclohexene; purity is unknown
Reliability	:	(2) valid with restrictions Verschueren (1983), Handbook of Environmental Data on Organic Chemicals 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

18.04.2007 (17)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	= 118.65 hPa at 25 °C
Decomposition	:	
Method	:	other (measured): not specified
Year	:	
GLP	:	no data
Test substance	:	
Test substance	:	CAS No. 110-83-8; cyclohexene; purity is unknown
Reliability	:	(2) valid with restrictions This robust summary has a reliability 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

18.04.2007 (3)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	= 2.86 at 20 °C
pH value	:	
Method	:	other (measured): not specified
Year	:	
GLP	:	no data
Test substance	:	
Test substance	:	CAS No. 110-83-8; cyclohexene; purity is unknown
Reliability	:	(2) valid with restrictions Data supplied by the experimental database associated with EPISuite. This robust summary has a reliability rating of 2 because the data was not reviewed for quality, however, the reference is associated with a peer-reviewed publication.
Flag	:	Critical study for SIDS endpoint

18.04.2007 (5)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	= 213 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: not specified
Year	:	
GLP	:	no data
Test substance	:	
Test substance	:	CAS No. 110-83-8; cyclohexene; purity is unknown
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are from a standard reference source.

Flag : Critical study for SIDS endpoint
18.04.2007 (18)

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	:	Sun light
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000 molecule/cm³
Rate constant	:	= .000000000000615237 cm³/(molecule*sec)
Degradation	:	= 50 % after .2 hour(s)
Deg. product	:	
Method	:	other (calculated): Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPI SuiteTM version 3.12
Year	:	
GLP	:	
Test substance	:	

Method	:	Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPI SuiteTM 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	:	Cyclohexene has the potential to volatilize to air, based on a relatively high vapor pressure, where it is subject to atmospheric oxidation. In air, cyclohexene can react with photosensitized oxygen in the form of hydroxyl radicals (OH-). The computer program AOPWIN (atmospheric oxidation program for Microsoft Windows) (EPI SuiteTM, 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. Based on a 12-hour day, a rate constant of 6.15 E-13 cm3/molecule*sec, and an OH- concentration of 1.5 E6 OH-/cm3, cyclohexene has a calculated half-life in air of 0.174 days or 2.086 hours of daylight.
Test substance	:	CAS No. 110-83-8; cyclohexene; purity is unknown
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

19.04.2007 (16)

Type	:	water
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight

Test condition	:	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, 1982).

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 and unsaturated hydrocarbons do not absorb light above 290 nm. Consequently, cyclohexene is not subject to photolytic processes in the aqueous environment.

Test substance : CAS No. 110-83-8; cyclohexene; purity is unknown
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
19.04.2007 (6) (19)

3.1.2 STABILITY IN WATER

Deg. product :
Method : other: Technical Discussion
Year :
GLP : no data
Test substance :

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. Cyclohexene is resistant to hydrolysis because it lacks a functional group that is hydrolytically reactive and Harris (1982) identifies hydrocarbons as generally resistant to hydrolysis. Therefore, hydrolysis will not contribute to the removal of cyclohexene from the environment.
Test substance : CAS No. 110-83-8; cyclohexene; purity is unknown
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
19.04.2007 (4) (7)

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

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	:	2003

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 3.04 program. Measured input values were also used where available and obtained from the EPIWIN database. 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, sediment, suspended sediment, biota).

Input values used:
Molecular mass = 82.15 g/mol
Water solubility = 213 mg/L
Vapour pressure = 11,865 Pa
log Kow = 2.86
Melting point = -103.5 deg C

Result :

Air - 99.82%
Water - 0.11%
Soil - 0.07%
Sediment - <0.01%
Suspended Sed - <0.01%
Biota - <0.01%

Test substance : CAS No. 110-83-8; cyclohexene; purity is unknown

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

19.04.2007 (8)

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	:	2003

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 3.04 program. Measured input values were also used where available and obtained from the EPIWIN database. 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 = 82.15 g/mol
Water solubility = 213 mg/L
Vapour pressure = 11,865 Pa
log Kow = 2.86
Melting point = -103.5 deg C

Degradation half-lives:

Air - 2.09 hrs
Water - 360 hrs
Soil - 720 hrs
Sediment - 7200 hrs

This model was run assuming a default emission rate of 1000 kg/hr into each of the air, water, and soil compartments.

Result :

Air - 3.0%
Water - 78.5%
Soil - 17.3%
Sediment - 1.2%

Test substance : CAS No. 110-83-8; cyclohexene; purity is unknown
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
19.04.2007 (8)

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic
Inoculum : activated sludge
Contact time : 28 day(s)
Degradation : = 0 (±) % after 28 day(s)
Result : under test conditions no biodegradation observed
Deg. product :
Method : other: Modified MITI test (Comparable to OECD 301C)
Year : 1992
GLP : no data
Test substance :

Test condition : Concentration of the test substance was 100 mg/l, with a concentration of inoculum of 30 mg/l. The source of the inoculum was non-acclimated activated sludge.Results of the study were based on BOD.
Test substance : CAS No. 110-83-8; cyclohexene; purity is unknown
Reliability : (2) valid with restrictions
The study was performed following acceptable guidlines, however, the data were not retrieved an reviewed for quality.
Flag : Critical study for SIDS endpoint
19.04.2007 (2)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

Species	:	Cyprinus carpio (Fish, fresh water)
Exposure period	:	28 day(s) at °C
Concentration	:	100 µg/l
BCF	:	= 12 - 38
Elimination	:	
Method	:	other: Bioconcetration Test
Year	:	2002
GLP	:	no data
Test substance	:	
Method	:	Test followed Japanese test guidelines. Lipid content of the fish was 2.71% at start of test, 2.21% at end of testing. Two concentrations of test substance were tested: 100 ug/L and 10 ug/L. No additional details for the test were included, remarks were available in Japanese only.
Result	:	BCF for test: 100 ug/l = 12 to 38 10 ug/l = 23 to 45 Low potential to bioconcentrate.
Test substance	:	CAS No. 110-83-8; cyclohexene; purity is unknown
Reliability	:	(2) valid with restrictions This robust summary was given a reliability rating of 2 because the data were not retrieved and reviewed for quality. The data were reported by the Japanese National Institute of Technology and Evaluation and are believed to be reliable.

23.04.2007 (2)

Species	:	other: see remark
Exposure period	:	at 25 °C
Concentration	:	
BCF	:	= 31.8
Elimination	:	
Method	:	other: Calculated
Year	:	2003
GLP	:	
Test substance	:	
Remark	:	A log bioconcentration factor (BCF) of 1.502 is calculated (BCF = 31.78). With respect to a log Kow = 2.86, which was used to calculate the BCF, cyclohexene in the aquatic environment is expected to have a low potential to bioaccumulate.
Test substance	:	CAS No. 110-83-8; cyclohexene; purity is unknown
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

19.04.2007 (16)

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	
Species	:	Oryzias latipes (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	> 10 measured/nominal
Limit test	:	
Analytical monitoring	:	no data
Method	:	other: Japanese guideline
Year	:	
GLP	:	no data
Test substance	:	
Remark	:	Study reported by the Japanese National Institute of Technology and Evaluation on their website. No other information regarding the study was reported. Remarks were available, but only in Japanese.
Test substance	:	CAS No. 110-83-8; cyclohexene; purity is unknown
Reliability	:	(2) valid with restrictions This robust summary was given a reliability rating of 2 because the data were not retrieved and evaluated for quality, however, the data were reported by a reliable source.
Flag	:	Critical study for SIDS endpoint

23.04.2007 (2)

Type	:	
Species	:	other: freshwater fish
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	= 7.6 calculated
Method	:	other: ECOSAR Computer Model
Year	:	
GLP	:	
Test substance	:	
Method	:	ECOSAR version 0.99h, U.S. 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 :

Calculated 96-hr LC50 for fish = 7.6 mg/L

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 EPIWIN computer model (2). KOWWIN also has a database of experimental Kow values (EXPKOW.DB).

The ECOSAR program was run using cyclohexene with a Kow of 2.86.

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

2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

Test substance : CAS No. 110-83-8; cyclohexene; purity is unknown

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

23.04.2007 (1)

Type : static
Species : Oncorhynchus kisutch (Fish, fresh water, marine)
Exposure period : 96 hour(s)
Unit : mg/l
LC50 : > 100 measured/nominal
Limit test : no
Analytical monitoring :
Method : other: not reported
Year : 1974
GLP : no
Test substance :

Remark : The study was performed in open vessels with full aeration in 30 ppt artificial seawater made with Instant Ocean brand seasalts. Fish were not fed during the experiment. Test tanks were 95 liter tanks containing 75 liters of water. The test substance was added to the test tank via a syringe to simulate an oil spill.

Loading of the test tank was adjusted to provide less than 1g of fish per liter of seawater. Cyclohexene was tested at 100 and 50 ppm. Fish were observed to "spasm" at both concentrations of cyclohexene upon additiona of the test substance to the water. Fish returned to "normal" after a short time interval (2 to 4 hours). No significant mortality was noted in the test.

Test substance : CAS No. 110-83-8; cyclohexene; purity is unknown

Reliability : (3) invalid
This robust summary was given a reliability rating of 3 because the study was performed in open test vessels with full aeration. Given the volatility of the test substance, an open vessel is not an appropriate test design.

23.04.2007 (13)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	
Species	:	Daphnia sp. (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
EC50	:	= 8.7 calculated
Method	:	other: ECOSAR Computer Model
Year	:	
GLP	:	
Test substance	:	
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 EPIWIN computer model (2). KOWWIN also has a database of experimental Kow values (EXPKOW.DB). The ECOSAR program was run using cyclohexene with a Kow of 2.86. 1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92. 2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Test substance	:	CAS No. 110-83-8; cyclohexene; purity is unknown
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

23.04.2007 (1)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	other algae: Pseudokirchneriella subcapitata
Endpoint	:	
Exposure period	:	96 hour(s)
Unit	:	mg/l
EC50	:	= 5.8 calculated
ChV	:	= 1 calculated
Method	:	other: ECOSAR Computer Model
Year	:	
GLP	:	
Test substance	:	
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 EPIWIN computer model (2). KOWWIN also has a database of experimental Kow values (EXPKOW.DB). The ECOSAR program was run using cyclohexene with a Kow of 2.86. 1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.

2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

Test substance : CAS No. 110-83-8; cyclohexene; purity is unknown

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

23.04.2007 (1)

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	:	Crj: CD(SD)
Sex	:	male/female
Number of animals	:	5
Vehicle	:	other: corn oil
Doses	:	0, 500, 1000, and 2000 mg/kg bw
Method	:	OECD Guide-line 401 "Acute Oral Toxicity"
Year	:	2002
GLP	:	yes
Test substance	:	other TS
Remark	:	Doses were 0, 500, 1000, and 2000 mg/kg bw for both sexes.
Result	:	LD50 value was greater than 1,000 mg/kg bw. Each 3 of 5 animals of male and female rats at 2,000 mg/kg bw showed abnormal gait, adoption of a prone position, salivation, piloerection and tremor, and then died within 3 days after dosing. Hypoactivity was observed in all male and female rats given the test substance. Lacrimation was also observed in both sexes just after dosing at 1,000 mg/kg bw and more. Necropsy of the dead animals revealed pulmonary congestion.

Mortality:

Dose(mg/kgbw)		0	500	1000	2000
No.of animals	5	5	5	5	
No.of death Male	0	0	0	3	
Female	0	0	0	3	

Source	:	Research Institute for Animal Science in Biochemistry and Toxicology Sagamihara Kanagawa
Test substance	:	Purity: 98.6%
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

06.10.2006 (9)

5.1.2 ACUTE INHALATION TOXICITY

Type	:	other: Lethal concentration
Value	:	> 6370 ppm
Species	:	rat
Strain	:	no data
Sex	:	no data
Number of animals	:	
Vehicle	:	no data
Doses	:	
Exposure time	:	4 hour(s)
Method	:	other
Year	:	
GLP	:	no data
Test substance	:	no data
Remark	:	Value: > 6370 ppm (> 21388 mg/m3)
Result	:	Toxic effects: Tremor and ataxia.

Source	:	Research Institute for Animal Science in Biochemistry and Toxicology Sagamihara Kanagawa

09.10.2006 (14)

5.1.3 ACUTE DERMAL TOXICITY

Type	:	LD50
Value	:	> 20 ml/kg bw
Species	:	guinea pig
Strain	:	no data
Sex	:	no data
Number of animals	:	
Vehicle	:	no data
Doses	:	
Method	:	other
Year	:	
GLP	:	no data
Test substance	:	no data
Result	:	Details of toxic effects were not reported other than lethal dose value.
Source	:	Research Institute for Animal Science in Biochemistry and Toxicology Sagamihara Kanagawa

06.10.2006 (15)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

Type	:	
Species	:	rat
Sex	:	male/female
Strain	:	other: Crj:CD(SD)IGS
Route of admin.	:	gavage
Exposure period	:	Males: 48 days; Females: 42-53 days from 14 days before mating to day 4 of lactation
Frequency of treatm.	:	Once a day
Post exposure period	:	None
Doses	:	50, 150, 500 mg/kg bw
Control group	:	yes, concurrent vehicle
NOAEL	:	= 50 mg/kg bw
Method	:	OECD combined study TG422
Year	:	2002
GLP	:	yes
Test substance	:	other TS
Remark	:	This study was conducted to examine both repeated dose toxicity and

reproductive/developmental toxicity as an OECD screening combined study (Test guideline: 422).
Study design:
Vehicle: Corn oil
Clinical observation performed and frequency: General condition was observed once a day, body weights were determined at days 1 (before dosing),8, 15, 22, 29, 36, 43 and 49 of treatment for males and at days 1, 8 and 15 of treatment and at days 0, 7, 14, and 20 of gestation period and at days 0 and 4 of lactation period and at autopsy for females, food consumption was determined at days 1, 8, 15, 22, 29, 36, 43 and 48 of treatment for males and at days 1,8 and 15 of treatment and at days 0, 7, 14 and 20 of gestation period and at days 0 and 4 of lactation for females, but food consumption were not determined during mating period for males and females.
For 5 males per group, urinalysis was carried out at 43-48 days of administration period. For all males and all females after childbirth, hematology and biochemistry were carried out at time of necropsy after 49 days for males and at 5 days after delivery for females. Organs examined at necropsy.
Organ weight: Brain, liver, kidney, spleen, adrenal, thymus, testis and epididymis
Microscopic examination: Brain, pituitary, thymus, thyroid, parathyroid, adrenal, spleen, heart, thoracic aorta, tongue, esophagus, stomach, liver, pancreas, duodenum, jejunum, ileum, cecum, colon, rectum, larynx, trachea, lung, kidney, urinary bladder, testis, epididymis, prostate, seminal vesicle, ovary, uterus, vagina, eye, harderian gland, mammary gland, skin, sternum, femur, spinal cord, skeletal muscle, mesentery lymph node, mandibular lymph node, submandibular gland, sublingual gland, parotid gland, ischiadic nerve, bone marrow, Statistical methods: Dunnett's test for continuous data and Steel test for quantal data.

Result **:** Mortality: There was no mortality related to the test substance treatment.
Clinical signs: Salivation was apparent in three animals of 150 mg/kg bw group and in twelve animals of 500 mg/kg bw group for males and in two animals of 150 mg/kg bw group and twelve animals of 500 mg/kg bw group for females. Although the grades of salivation were not reported, the sign was observed for about 5 minutes after dosing at 150 mg/kg bw, and for 30 minutes to 5 hours after dosing at 500 mg/kg bw during treatment period. In addition, lacrimation was observed in two animals of 500 mg/kg bw group for males and in one animal each of 150 and 500 mg/kg bw groups for females. The onsets and grades of lacrimation were not reported.
Body weight: No statistically significant changes for males and females.
Food consumption: No effects for males and females.
Urinalysis: No statistically significant changes.
Hematology: No effects for males and females
Blood biochemistry: Males: Decreases in triglyceride in 150 and 500 mg/kg bw groups, increases in total bilirubin in 500 mg/kg bw group, and total bile acid in 150 and 500 mg/kg bw.

Dose (mg/kg bw)	0	50	150	500
No.of animals	12	11	12	12
Triglyceride (mg/dL) Mean	39.2	6.8	27.7	22.5
SD	22.4	18.8	16.7	7.7
T.bilirubin (mg/dL) Mean	0.03	0.04	0.05	0.05*
SD	0.01	0.01	0.01	0.01
T.bile acid (umol/L) Mean	18.8	20.8	39.9*	32.6
SD	15.0	16.6	21.0	25.5

Note: *, P<0.05

Females: Increase in total bile acid in 50, 150, and 500 mg/kg bw.

Dose (mg/kg bw)		0	50	150	500
No. of animals	10	10	10	10	

T.bile acid (umol/L) Mean	19.3	49.2*	31.2	82.2*	
SD	8.6	28.8	19.7	81.1	

Note: *, p<0.05

Necropsy and histopathology: No adverse effects for males and females
Organ weights: Males: Increase in a relative kidney weight in 500 mg/kg bw group.

Dose (mg/kg bw)		0	50	150	500
No.of animals	12	11	12	12	
Kidney Absolute (g) Mean	3.21	3.09	3.20	3.31	
SD	0.33	0.27	0.27	0.27	
Relative (g%) Mean	0.652	0.619	0.667	0.705*	
SD	0.057	0.031	0.059	0.053	

Note: *, p<0.05

Females: No statistically significant changes.

Histopathology: No changes related to test substance.

Source : Research Institute for Animal Science in Biochemistry and Toxicology Sagamihara Kanagawa
Test substance : Purity: 98.6%
Conclusion : Increase in total bile acid noted in females of 50 mg/kg bw was not considered as an adverse effect because of no accompanying changes. Therefore, based on salivation observed at 150 mg/kg bw, the NOAEL for repeated dose toxicity was considered to be 50 mg/kg bw/day.
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
06.10.2006 (10)

5.5 GENETIC TOXICITY 'IN VITRO'

Type : Ames test
System of testing : Test spicies/strain: Salmonella typhimurium TA100, TA1535, TA98, TA1537, Escherichia coli WP2 uvrA
Test concentration : See "Remark"
Cycotoxic concentr. :
Metabolic activation : with and without
Result : negative
Method : other: Chemical Substance Control Law of Japan and OECD Test Guideline 471
Year : 2002
GLP : yes
Test substance : other TS

Remark : Procedures: Pre-incubation method
Solvent: Ethanol
Dosage of each strain with or without S9
-S9 mix: 0, 19.5, 39.1, 78.1, 156, 313, 625, 1250 ug/plate (TA100, TA1535, TA98, TA1537); 0, 78.1, 156, 313, 625, 1250, 2500, 5000 ug/plate (WP2 uvrA)
+S9 mix: 0, 19.5, 39.1, 78.1, 156, 313, 625, 1250 ug/plate (all strain)
*Maximum concentration was established based on the result of the preliminary test up to 5000 ug/plate. In this test, the growth inhibition was observed at 1250 ug/plate and more with and without S9 mix in Salmonella typhimurium TA100, TA98, TA1535, TA1537 and with S9 mix in Escherichia coli WP2 uvrA.
Positive control: without S9 mix:
2-(2-furyl)-3-(5-nitro-2-furyl)acrylamide (TA100, TA98, WP2 uvrA), Sodium azide (TA 1535), 2-methoxy-6-chloro-9-[3-(2-chloroethyl)-

aminopropylamino]acriine 2HCl
with S9 mix: Benzo[a]pyrene (TA100, TA98), 2-aminoanthracene (TA1535, WP2 uvrA, TA1537)
S9: Rat liver, induced with phenobarbital and 5,6-benzoflavone
Plates/test: 3

Result : There were no precipitations in any test concentration.
Cytotoxic concentration: Growth inhibition was observed at 625 ug/plate or more with or without S9 mix in Salmonella typhimurium TA100, TA1535, TA98, TA1537, and at 1250 ug/plate or more with S9 in Escherichia coli WP2 uvrA.
Genotoxic effects:
With metabolic activation: negative
Without metabolic activation: negative

Source : Research Institute for Animal Science in Biochemistry and Toxicology Sagamihara Kanagawa

Test substance : Purity: 98.63%

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

06.10.2006 (11)

Type : Chromosomal aberration test

System of testing : Type of cell used: Chinese hamster lung(CHL/IU) cell

Test concentration : 0, 100, 150, 200, 250, 300, 350, 400 ug/mL

Cycotoxic concentr. : 400 ug/mL

Metabolic activation : with and without

Result : negative

Method : other: Chemical Substances Control Law of Japan and OECD Test Guideline 473

Year : 2002

GLP : yes

Test substance : other TS

Remark : Solvent: Ethanol
S9: Rat liver, induced with phenobarbital and 5,6-benzoflavone
Plates/test: 2
The maximum concentration was established, based on the growth inhibition test. In this test, 50% growth inhibition was observed between 250 and 300 ug/mL for short-term treatment and continuous treatment with or without S9.

Result : No increase in chromosomal aberrations was observed after short-term or continuous treatment with or without S9 mix.
Cell toxicity was observed at 400 ug/mL after continuous treatments for 24 and 48 hrs.

Source : Research Institute for Animal Science in Biochemistry and Toxicology Sagamihara Kanagawa

Test substance : Purity: 98.63%

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

06.10.2006 (12)

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

Type : other

Species	:	rat
Sex	:	male/female
Strain	:	other: Crj:CD(SD)IGS
Route of admin.	:	gavage
Exposure period	:	Males:48 days, females:42-53 days from 14 days before mating to day 4 of lactation
Frequency of treatm.	:	once a day
Premating exposure period		
Male	:	14 days
Female	:	14 days
Duration of test	:	Males: 49 days; Females: from 14 days before day 5 of lactation
No. of generation studies	:	
Doses	:	50, 150, 500 mg/kgbw
Control group	:	yes, concurrent vehicle
NOAEL parental	:	= 500 mg/kg bw
NOAEL F1 offspring	:	= 500 mg/kg bw
Result	:	NOAEL Parental = 500 mg/kg bw; NOAEL F1 Offspr. = 500 mg/kg bw
Method	:	other: OECD Test guideline 422
Year	:	2002
GLP	:	yes
Test substance	:	other TS

Remark : This study was conducted to examine both repeated dose toxicity and reproductive/developmental toxicity as an OECD screening combined study (Test guideline: 422).
Study design:
Vehicle: Corn oil
Clinical observation performed and frequency: General condition was observed once a day, body weights were determined at days 1 (before dosing), 8, 15, 22, 29, 36, 43 and 49 of treatment for males and at days 1, 8 and 15 of treatment and at days 0, 7, 14, and 20 of gestation period and at days 0 and 4 of lactation period and at autopsy for females, food consumption was determined at days 1, 8, 15, 22, 29, 36, 43 and 48 of treatment for males and at days 1,8 and 15 of treatment and at days 0, 7, 14 and 20 of gestation period and at days 0 and 4 of lactation for females, but food consumption were not determined during mating period for males and females.
For 5 males per group, urinalysis was carried out at 43-48 days of administration period. For all males and all females after childbirth per group, hematology and biochemistry were carried out at time of necropsy after 49 days for males and at 5 days after delivery for females. Organs examined at necropsy.
Organ weight: Brain, liver, kidney, spleen, adrenal, thymus, testis and epididymis
Microscopic examination: Brain, pituitary, thymus, thyroid, parathyroid, adrenal, spleen, heart, thoracic aorta, tongue, esophagus, stomach, liver, pancreas, duodenum, jejunum, ileum, cecum, colon, rectum, larynx, trachea, lung, kidney, urinary bladder, testis, epididymis, prostate, seminal vesicle, ovary, uterus, vagina, eye, harderian gland, mammary gland, skin, sternum, femur, spinal cord, skeletal muscle, mesentery lymph node, mandibular lymph node, submandibular gland, sublingual gland, parotid gland, ischiadic nerve, bone marrow.
Reproductive and developmental parameters: No.of pairs with successful copulation, No. of pregnant females, copulation index (No. of pairs with successful copulation/No. of pairs mated x 100), fertility index (No. of pregnant animals/No.of animals with successful copulation x 100), estrous cycle, No. of dams delivered live pups, duration of gestation, No. of total corpora lutea, No. of total implants, No. of total pups born, No. of total live pups born, sex ratio, No. of total dead pups, No. of total cannibalism, gestation index (No. of females with live pups/No. of pregnant females x 100), implantation index (No. of implants/No.of corpora lutea x 100),

delivery index (No. of pups born/No. of implants x 100), live birth index (No. of live pups born/No. of pups born x 100), and viability index on day 4 (No. of live pups on day 4 after birth/No. of live pups born x 100). Statistical methods: Dunnett's test for continuous data and Steel test for quantal data.

Result : Mortality: There was no mortality related to the test substance treatment.
Clinical signs: Salivation was apparent in three animals of 150 mg/kg bw group and in twelve animals of 500 mg/kg bw group for males and in two animals of 150 mg/kg bw group and twelve animals of 500 mg/kg bw group for females. Although the grades of salivation were not reported, the sign was observed for about 5 minutes after dosing at 150 mg/kg bw, and for 30 minutes to 5 hours after dosing at 500 mg/kg bw during treatment period. In addition, lacrimation was observed in two animals of 500 mg/kg bw group for males and in one animal each of 150 and 500 mg/kg bw groups for females. The onsets and grades of lacrimation were not reported.
Body weight: No statistically significant changes for males and females.
Food consumption: No effects for males and females.
Urinalysis: No statistically significant changes.
Hematology: No effects for males and females
Blood biochemistry:
Males: Decreases in triglyceride in 150 and 500 mg/kg bw groups, increases in total bilirubin in 500 mg/kg bw group, and total bile acid in 150 and 500 mg/kg bw.
Females: Increase in total bile acid in 50, 150, and 500 mg/kg bw.
Necropsy and histopathology: No adverse effects for males and females.
Organ weights:
Males: Increase in a relative kidney weight in 500 mg/kg bw group.
Females: No statistically changes.

Histopathology: No changes related to test substance.
Reproductive and developmental parameters: No effects observed on reproductive performance in males and females given each dose, and developmental performance of the newborns.

Dose(mg/kg bw)		0	50	150	500
No. of pairs mated	12	12	12	12	
No. of pairs copulated	12	11	12	12	
No. of pregnant females		11	10	10	10
Copulation index (%)	100.0	91.7	100.0	100.0	
Fertility index (%)	91.7	90.9	83.3	83.3	
No. of dams observed	11	10	10	10	
No. of dams delivered live pups	11	10	10	10	
Duration of gestation:					
Mean	22.5	22.2	22.3	22.5	
SD	0.5	0.4	0.5	0.5	
No. of total corpora lutea:					
Mean	19.2	17.4	18.4	20.1	
SD	2.6	3.3	3.2	3.8	
No. of total implants:					
Mean	13.7	14.4	14.3	14.3	
SD	3.0	1.6	1.5	1.6	
No. of total pups born:					
Mean	12.8	13.4	13.5	12.5	
SD	3.5	1.6	2.1	2.2	
Sex ratio: Mean	0.80	1.32	1.14	0.81	
SD	0.23	0.68	1.60	0.56	
No. of total live pups on day 4					
Male: Mean	5.5	6.9	6.7	5.0	
SD	2.2	1.9	2.4	2.0	
Female: Mean	6.8	6.2	6.7	7.2	
SD	2.8	1.9	2.4	2.0	
No. of total dead pups:					

	Mean	0.3	0.1	0.1	0.0
	SD	0.6	0.3	0.3	0.0
Gestation index (%):		100.0	100.0	100.0	100.0
Implantation index (%):					
	Mean	73.2	84.1	79.0	72.9
	SD	20.3	9.7	10.6	13.1
Delivery index (%):					
	Mean	93.2	93.8	97.3	90.0
	SD	11.9	6.1	4.7	10.3
Live birth index (%):					
	Mean	98.0	99.3	96.9	97.0
	SD	4.7	2.3	9.7	9.5
Viability index day 4					
Male:	Mean	90.9	95.3	100.0	96.7
	SD	30.2	10.0	0.0	10.5
Female:	Mean	88.6	100.0	98.3	98.3
	SD	29.8	0.0	5.3	5.3

Source : Research Institute for Animal Science in Biochemistry and Toxicology Sagamihara Kanagawa
Test substance : Purity: 98.6%
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
11.10.2006 (10)

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species : rat
Sex : male/female
Strain : other: Crj:CD(SD)IGS
Route of admin. : gavage
Exposure period : Males:48 days, females:42-53 days from 14 days before mating to day 4 of lactation
Frequency of treatm. : once a day
Duration of test : Males: 49 days; Females: from 14 days before day 5 of lactation
Doses : 50, 150, 500 mg/kgbw
Control group : yes, concurrent vehicle
other: NOAEL Parental : = 500 mg/kg bw
other: NOAEL F1 Offspr. : = 500 - mg/kg bw
Result : NOAEL Parental = 500 mg/kg bw; NOAEL F1 Offspr. = 500 mg/kg bw
Method : other: OECD Test guideline 422
Year : 2002
GLP : yes
Test substance : other TS

Remark : This study was conducted to examine both repeated dose toxicity and reproductive/developmental toxicity as an OECD screening combined study (Test guideline: 422).
Study design:
Vehicle: Corn oil
Clinical observation performed and frequency: General condition was observed once a day, body weights were determined at days 1 (before dosing), 8, 15, 22, 29, 36, 43 and 49 of treatment for males and at days 1, 8 and 15 of treatment and at days 0, 7, 14, and 20 of gestation period and at days 0 and 4 of lactation period and at autopsy for females, food consumption was determined at days 1, 8, 15, 22, 29, 36, 43 and 48 of treatment for males and at days 1,8 and 15 of treatment and at days 0, 7, 14 and 20 of gestation period and at days 0 and 4 of lactation for females, but food consumption were not determined during mating period for males and females.

For 5 males per group, urinalysis was carried out at 43-48 days of administration period. For all males and all females after childbirth per group, hematology and biochemistry were carried out at time of necropsy after 49 days for males and at 5 days after delivery for females. Organs examined at necropsy.
Organ weight: Brain, liver, kidney, spleen, adrenal, thymus, testis and epididymis
Microscopic examination: Brain, pituitary, thymus, thyroid, parathyroid, adrenal, spleen, heart, thoracic aorta, tongue, esophagus, stomach, liver, pancreas, duodenum, jejunum, ileum, cecum, colon, rectum, larynx, trachea, lung, kidney, urinary bladder, testis, epididymis, prostate, seminal vesicle, ovary, uterus, vagina, eye, harderian gland, mammary gland, skin, sternum, femur, spinal cord, skeletal muscle, mesentery lymph node, mandibular lymph node, submandibular gland, sublingual gland, parotid gland, ischiadic nerve, bone marrow.
Reproductive and developmental parameters: No.of pairs with successful copulation, No. of pregnant females, copulation index (No. of pairs with successful copulation/No. of pairs mated x 100), fertility index (No. of pregnant animals/No.of animals with successful copulation x 100), estrous cycle, No. of dams delivered live pups, duration of gestation, No. of total corpora lutea, No. of total implants, No. of total pups born, No. of total live pups born, sex ratio, No. of total dead pups, No. of total cannibalism, gestation index (No. of females with live pups/No. of pregnant females x 100), implantation index (No. of implants/No.of corpora lutea x 100), delivery index (No. of pups born/No. of implants x 100), live birth index (No. of live pups born/No. of pups born x 100), and viability index on day 4 (No. of live pups on day 4 after birth/No. of live pups born x 100). Statistical methods: Dunnett's test for continuous data and Steel test for quantal data.

Result **:** There was no mortality related to the test substance treatment. Salivation was apparent in three animals of 150 mg/kg bw group and in twelve animals of 500 mg/kg bw group for males and in two animals of 150 mg/kg bw group and twelve animals of 500 mg/kg bw group for females. Although the grades of salivation were not reported, the sign was observed for about 5 minutes after dosing at 150 mg/kg bw, and for 30 minutes to 5 hours after dosing at 500 mg/kg bw during treatment period. In addition, lacrimation was observed in two animals of 500 mg/kg bw group for males and in one animal each of 150 and 500 mg/kg bw groups for females. The onsets and grades of lacrimation were not reported.

There were no statistically significant changes in body weight, food consumption, urinalysis and hematology for males and females.

Blood biochemistry:
Males: Decreases in triglyceride in 150 and 500 mg/kg bw groups, increases in total bilirubin in 500 mg/kg bw group, and total bile acid in 150 and 500 mg/kg bw.
Females: Increase in total bile acid in 50, 150, and 500 mg/kg bw.
Necropsy and histopathology: No adverse effects for males and females.
Organ weights:
Males: Increase in a relative kidney weight in 500 mg/kg bw group.
Females: No statistical changes.

Histopathology: No changes related to test substance.
Reproductive and developmental parameters: No effects observed on reproductive performance in males and females given each dose, and developmental performance of the newborns.

Dose(mg/kg bw)			0	50	150	500
No. of total pups born:						
	Mean	12.8	13.4	13.5	12.5	
	SD	3.5	1.6	2.1	2.2	
Sex ratio:	Mean	0.80	1.32	1.14	0.81	

	SD	0.23	0.68	1.60	0.56
No. of total live pups on day 4					
Male:	Mean	5.5	6.9	6.7	5.0
	SD	2.2	1.9	2.4	2.0
Female:	Mean	6.8	6.2	6.7	7.2
	SD	2.8	1.9	2.4	2.0
No. of total dead pups:					
	Mean	0.3	0.1	0.1	0.0
	SD	0.6	0.3	0.3	0.0
Viability index day 4					
Male:	Mean	90.9	95.3	100.0	96.7
	SD	30.2	10.0	0.0	10.5
Female:	Mean	88.6	100.0	98.3	98.3
	SD	29.8	0.0	5.3	5.3

Source : Research Institute for Animal Science in Biochemistry and Toxicology Sagamihara Kanagawa
Test substance : Purity: 98.6%
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
09.10.2006 (10)

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

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

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10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

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V   IUCLID-Export V4.00
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NL  GBR
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B003 DS_ADMIN_TAB
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F003 10-07-2007
F101 U.S. EPA - HPV Challenge Program
F102 A35-02
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F004 1545 Route 22 East
F005 Annadale, New Jersey
F006 08801-3059
F008 A31-024
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B203 PC_DENSITY_TAB
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F009 .81
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B204 PC_VAPOUR_TAB
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F030 C14-001
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F008 F01-04
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F009 F02-05: Calculated values using AOPWIN version 1.89, a subroutine of the
* computer program EPI SuiteTM version 3.12
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B302 EN_STABILITY_IN_WATER_TAB
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B305 EN_TRANSPORT_TAB
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F007 F20-07
F008 F22-01: air - sediment(s) - soil - water
F009 F21-01: Calculation according Mackay, Level III
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F007 F20-05
F008 F22-01: air - biota - sediment(s) - soil - water
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F020 F30-04
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F009 F34-06: Calculated
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B401 EC_FISHTOX_TAB
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F010 E03-05: ECOSAR Computer Model
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F014 E05-02
F021 A02-03
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F010 E03-05: Japanese guideline
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F013 E04-02
F014 E05-02
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F032 A03-02
F045 E35-02
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B402 EC_DAPHNIATOX_TAB
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B403 EC_ALGAETOX_TAB
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F014 E05-02
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F009 T02-24
F010 T03-02
F011 2002
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F019 T24-03
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F022 T23-49
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F018 A03-02
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F023 T52-002
F024 T23-47
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F011 T25-03
F012 T26-45
F013 2002
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* of lactation
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F016 None
F017 50, 150, 500 mg/kg bw
F018 T27-05
F019 A02-03
F020 50
F022 T28-03
F029 A03-03
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B509 TO_GENETIC_IN_VITRO_TAB
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F008 T30-01
F009 T31-18: Chemical Substance Control Law of Japan and OECD Test Guideline
* 471
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F011 Test spicies/strain: Salmonella typhimurium TA100, TA1535, TA98, TA1537,
* Escherichia coli WP2 uvrA

F012 T32-03
F013 T33-02
F014 A03-03
F015 See "Remark"
EOR
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F017 2
F007 A01-03
F008 T30-20
F009 T31-18: Chemical Substances Control Law of Japan and OECD Test Guideline
* 473
F010 2002
F011 Type of cell used: Chinese hamster lung(CHL/IU) cell
F012 T32-03
F013 T33-02
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F018 400 ug/mL
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F009 T02-24
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F012 T25-03
F036 Males:48 days, females:42-53 days from 14 days before mating to day 4 of
* lactation
F013 T40-05: OECD Test guideline 422
F014 2002
F015 once a day
F016 14 days
F017 14 days
F018 Males: 49 days; Females: from 14 days before day 5 of lactation
F019 50, 150, 500 mg/kgbw
F020 T27-05
F021 A02-03
F022 500
F024 T43-02
F025 A02-03
F026 500

F028 T43-02
F035 A03-03
F055 NOAEL Parental = 500 mg/kg bw; NOAEL F1 Offspr. = 500 mg/kg bw
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F011 T25-03
F012 T44-03: OECD Test guideline 422
F013 2002
F014 Males: 49 days; Females: from 14 days before day 5 of lactation
F015 Males:48 days, females:42-53 days from 14 days before mating to day 4 of
* lactation
F016 once a day
F017 50, 150, 500 mg/kgbw
F018 T27-05
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F032 T58-007: NOAEL Parental
F033 A02-03
F034 500
F036 T43-02
F037 T58-007: NOAEL F1 Offspr.
F038 A02-03
F039 500
F041 T43-02
F047 NOAEL Parental = 500 mg/kg bw; NOAEL F1 Offspr. = 500 mg/kg bw
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B601 TEXT_TAB
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F010 2.1
F004 1
F005 RE
F006 U.S. Environmental Protection Agency (U.S. EPA) (2000). EPI SuiteTM,
* Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.
F007 U.S. Environmental Protection Agency (U.S. EPA) (2000). EPI SuiteTM,
* Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.
F020 261712
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* insufficient information available on the method and analytical procedure.
F007 This robust summary has a reliability rating of 2 because there is
* insufficient information available on the method and analytical procedure.
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F007 CAS No. 110-83-8; cyclohexene; purity is unknown
F020 261701
EOR
F002 518
F010 2.2
F004 1
F005 RE
F006 U.S. Environmental Protection Agency (U.S. EPA) (2000). EPI SuiteTM,
* Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.
F007 U.S. Environmental Protection Agency (U.S. EPA) (2000). EPI SuiteTM,
* Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.
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F006 This robust summary has a reliability rating of 2 because there is
* insufficient information available on the method and analytical procedure.
F007 This robust summary has a reliability rating of 2 because there is
* insufficient information available on the method and analytical procedure.
F020 261708
EOR
F002 518
F010 2.2
F004 1
F005 TS
F006 CAS No. 110-83-8; cyclohexene; purity is unknown
F007 CAS No. 110-83-8; cyclohexene; purity is unknown
F020 261702
EOR
F002 518
F010 2.3
F004 1
F005 RE
F006 Verschueren, K. (1983). Handbook of Environmental Data on Organic
* Chemicals, Second Edition. Van Nostrand Rienhold, New York
F007 Verschueren, K. (1983). Handbook of Environmental Data on Organic
* Chemicals, Second Edition. Van Nostrand Rienhold, New York
F020 261710
EOR

F002 518
F010 2.3
F004 1
F005 RL
F006 Verschueren (1983), Handbook of Environmental Data on Organic Chemicals
* 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 proc
F007 Verschueren (1983), Handbook of Environmental Data on Organic Chemicals
* 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 261709
EOR
F002 518
F010 2.3
F004 1
F005 TS
F006 CAS No. 110-83-8; cyclohexene; purity is unknown
F007 CAS No. 110-83-8; cyclohexene; purity is unknown
F020 261703
EOR
F002 518
F010 2.4
F004 1
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 261714
EOR
F002 518
F010 2.4
F004 1
F005 RL
F006 This robust summary has a reliability 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 of 2 because the data were not
* reviewed for quality, however, the reference is from a peer-reviewed
* handbook.
F020 261713
EOR
F002 518
F010 2.4
F004 1
F005 TS

F006 CAS No. 110-83-8; cyclohexene; purity is unknown
F007 CAS No. 110-83-8; cyclohexene; purity is unknown
F020 261704
EOR
F002 518
F010 2.5
F004 1
F005 RE
F006 Hansch, C., Leo, A., and Hoekman, D. (1995). Exploring QSAR -
* Hydrophobic, Electronic, and Steric Constants. American Chemical Society.
* Washington, DC, USA
F007 Hansch, C., Leo, A., and Hoekman, D. (1995). Exploring QSAR -
* Hydrophobic, Electronic, and Steric Constants. American Chemical Society.
* Washington, DC, USA
F020 261716
EOR
F002 518
F010 2.5
F004 1
F005 RL
F006 Data supplied by the experimental database associated with EPISuite.
* This robust summary has a reliability rating of 2 because the data was
* not reviewed for quality, however, the reference is associated with a
* peer-reviewed publication.
F007 Data supplied by the experimental database associated with EPISuite.
* This robust summary has a reliability rating of 2 because the data was
* not reviewed for quality, however, the reference is associated with a
* peer-reviewed publication.
F020 261715
EOR
F002 518
F010 2.5
F004 1
F005 TS
F006 CAS No. 110-83-8; cyclohexene; purity is unknown
F007 CAS No. 110-83-8; cyclohexene; purity is unknown
F020 261705
EOR
F002 518
F010 2.6.1
F004 1
F005 RE
F006 Yalkowsky S and Dannenfelser R (1992). Aquasol Database of Aqueous
* Solubility. Version 5. College of Pharmacy, University of Arizona, AZ,
* USA.
F007 Yalkowsky S and Dannenfelser R (1992). Aquasol Database of Aqueous
* Solubility. Version 5. College of Pharmacy, University of Arizona, AZ,
* USA.
F020 261718
EOR
F002 518
F010 2.6.1

F004 1
F005 RL
F006 This robust summary has a reliability rating of 2 because the data are
* from a standard reference source.
F007 This robust summary has a reliability rating of 2 because the data are
* from a standard reference source.
F020 261717
EOR
F002 518
F010 2.6.1
F004 1
F005 TS
F006 CAS No. 110-83-8; cyclohexene; purity is unknown
F007 CAS No. 110-83-8; cyclohexene; purity is unknown
F020 261706
EOR
F002 518
F010 3.1.1
F004 1
F005 RE
F006 Harris J (1982). Rate of Aqueous Photolysis. In: Handbook of Chemical
* Property Estimation Methods. Chapter 8. Edited by WJ Lyman, WF Reehl and
* DH Rosenblatt. McGraw-Hill Book Company, New York, NY, USA.
F007 Harris J (1982). Rate of Aqueous Photolysis. In: Handbook of Chemical
* Property Estimation Methods. Chapter 8. Edited by WJ Lyman, WF Reehl and
* DH Rosenblatt. McGraw-Hill Book Company, New York, NY, USA.
F020 261724
EOR
F002 518
F010 3.1.1
F004 1
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 261725
EOR
F002 518
F010 3.1.1
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 261723
EOR
F002 518
F010 3.1.1
F004 1
F005 TC

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, 1982).
**
** 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 and unsaturated
* hydrocarbons do not absorb light above 290 nm. Consequently, cyclohexene
* is not subject to photolytic processes in the aqueous environment.
F020 261722
EOR
F002 518
F010 3.1.1
F004 1
F005 TS
F006 CAS No. 110-83-8; cyclohexene; purity is unknown
F007 CAS No. 110-83-8; cyclohexene; purity is unknown
F020 261721
EOR
F002 518
F010 3.1.1
F004 2
F005 ME
F006 Calculated values using AOPWIN version 1.89, a subroutine of the computer
* program EPI SuiteTM version 3.12
**
** Indirect photodegradation, or atmospheric oxidation potential, is based
* on the structure-activity relationship methods developed by
F007 Calculated values using AOPWIN version 1.89, a subroutine of the computer
* program EPI SuiteTM 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 261727
EOR
F002 518
F010 3.1.1

F004 2
F005 RE
F006 U.S. Environmental Protection Agency (U.S. EPA) (2000). EPI SuiteTM,
* Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.
F007 U.S. Environmental Protection Agency (U.S. EPA) (2000). EPI SuiteTM,
* Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.
F020 261730
EOR
F002 518
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 261728
EOR
F002 518
F010 3.1.1
F004 2
F005 RM
F006 Cyclohexene has the potential to volatilize to air, based on a relatively
* high vapor pressure, where it is subject to atmospheric oxidation.
**
** In air, cyclohexene can react with photosensitized oxygen in the form of
* hydroxyl radicals (OH-).
F007 Cyclohexene has the potential to volatilize to air, based on a relatively
* high vapor pressure, where it is subject to atmospheric oxidation.
**
** In air, cyclohexene can react with photosensitized oxygen in the form of
* hydroxyl radicals (OH-). The computer program AOPWIN (atmospheric
* oxidation program for Microsoft Windows) (EPI SuiteTM, 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.
**
** Based on a 12-hour day, a rate constant of 6.15 E-13 cm3/molecule*sec,
* and an OH- concentration of 1.5 E6 OH-/cm3, cyclohexene has a calculated
* half-life in air of 0.174 days or 2.086 hours of daylight.
F020 261729
EOR
F002 518
F010 3.1.1
F004 2
F005 TS
F006 CAS No. 110-83-8; cyclohexene; purity is unknown
F007 CAS No. 110-83-8; cyclohexene; purity is unknown
F020 261726

EOR
F002 518
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 261734
EOR
F002 518
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 261735
EOR
F002 518
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 261733
EOR
F002 518
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. Cyclohexene is resistant to hydrolysis because it lacks a
* functional group that is hydrolytically reactive and Harris (1982)
* identifies hydrocarbons as generally resistant to hydrolysis. Therefore,
* hydrolysis will not contribute to the removal of cyclohexene from the
* environment.

F020 261731
EOR
F002 518
F010 3.1.2
F004 1
F005 TS
F006 CAS No. 110-83-8; cyclohexene; purity is unknown
F007 CAS No. 110-83-8; cyclohexene; purity is unknown
F020 261732
EOR
F002 518
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 3.04 program. Measured input values were also used
* where available and obtained from the EPIWIN database. 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 = 82.15 g/mol
** Water solubility = 213 mg/L
** Vapour pressure = 11,865 Pa
** log Kow = 2.86
** Melting point = -103.5 deg C
**
** Degradation half-lives:
**
** Air - 2.09 hrs
** Water - 360 hrs
** Soil - 720 hrs
** Sediment - 7200 hrs
**
** This model was run assuming a default emission rate of 1000 kg/hr into
* each of the air, water, and soil compartments.
F020 261736
EOR
F002 518
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 261740
EOR
F002 518
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 261739
EOR
F002 518
F010 3.3.1
F004 1
F005 RS
F006
** Air - 3.0%
** Water - 78.5%
** Soil - 17.3%
** Sediment - 1.2%
**
F007
** Air - 3.0%
** Water - 78.5%
** Soil - 17.3%
** Sediment - 1.2%
**
F020 261737
EOR
F002 518
F010 3.3.1
F004 1
F005 TS
F006 CAS No. 110-83-8; cyclohexene; purity is unknown
F007 CAS No. 110-83-8; cyclohexene; purity is unknown
F020 261738
EOR
F002 518
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 3.04 program. Measured input values were also used
* where available and obtained from the EPIWIN database. 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, sediment, suspended sediment,
* biota).
**
** Input values used:
** Molecular mass = 82.15 g/mol
** Water solubility = 213 mg/L
** Vapour pressure = 11,865 Pa
** log Kow = 2.86
** Melting point = -103.5 deg C
F020 261742
EOR
F002 518
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 261741
EOR
F002 518
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 261745
EOR
F002 518
F010 3.3.1
F004 2
F005 RS
F006
** Air - 99.82%
** Water - 0.11%
** Soil - 0.07%
** Sediment - <0.01%
** Suspended Sed - <0.01%
** Biota - <0.01%
**

F007
** Air - 99.82%
** Water - 0.11%
** Soil - 0.07%
** Sediment - <0.01%
** Suspended Sed - <0.01%
** Biota - <0.01%
**
F020 261744
EOR
F002 518
F010 3.3.1
F004 2
F005 TS
F006 CAS No. 110-83-8; cyclohexene; purity is unknown
F007 CAS No. 110-83-8; cyclohexene; purity is unknown
F020 261743
EOR
F002 518
F010 3.5
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 Internat
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 261749
EOR
F002 518
F010 3.5
F004 1
F005 RL
F006 The study was performed following acceptable guidlines, however, the data
* were not retrieved an reviewed for quality.
F007 The study was performed following acceptable guidlines, however, the data
* were not retrieved an reviewed for quality.
F020 261748
EOR
F002 518
F010 3.5
F004 1
F005 TC
F006 Concentration of the test substance was 100 mg/l, with a concentration of
* inoculum of 30 mg/l. The source of the inoculum was non-acclimated
* activated sludge.Results of the study were based on BOD.
F007 Concentration of the test substance was 100 mg/l, with a concentration of
* inoculum of 30 mg/l. The source of the inoculum was non-acclimated

* activated sludge.Results of the study were based on BOD.
F020 261747
EOR
F002 518
F010 3.5
F004 1
F005 TS
F006 CAS No. 110-83-8; cyclohexene; purity is unknown
F007 CAS No. 110-83-8; cyclohexene; purity is unknown
F020 261746
EOR
F002 518
F010 3.7
F004 1
F005 RE
F006 U.S. Environmental Protection Agency (U.S. EPA) (2000). EPI SuiteTM,
* Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.
F007 U.S. Environmental Protection Agency (U.S. EPA) (2000). EPI SuiteTM,
* Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.
F020 261753
EOR
F002 518
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 261752
EOR
F002 518
F010 3.7
F004 1
F005 RM
F006 A log bioconcentration factor (BCF) of 1.502 is calculated (BCF = 31.78).
* With respect to a log Kow = 2.86, which was used to calculate the BCF,
* cyclohexene in the aquatic environment is expected to have a low
* potential to bioaccumulate.
F007 A log bioconcentration factor (BCF) of 1.502 is calculated (BCF = 31.78).
* With respect to a log Kow = 2.86, which was used to calculate the BCF,
* cyclohexene in the aquatic environment is expected to have a low
* potential to bioaccumulate.
F020 261751
EOR
F002 518
F010 3.7
F004 1
F005 TS
F006 CAS No. 110-83-8; cyclohexene; purity is unknown
F007 CAS No. 110-83-8; cyclohexene; purity is unknown
F020 261750

EOR
F002 518
F010 3.7
F004 2
F005 ME
F006 Test followed Japanese test guidelines. Lipid content of the fish was
* 2.71% at start of test, 2.21% at end of testing. Two concentrations of
* test substance were tested: 100 ug/L and 10 ug/L. No additional details
* for the test were include
F007 Test followed Japanese test guidelines. Lipid content of the fish was
* 2.71% at start of test, 2.21% at end of testing. Two concentrations of
* test substance were tested: 100 ug/L and 10 ug/L. No additional details
* for the test were included, remarks were available in Japanese only.
F020 261762
EOR
F002 518
F010 3.7
F004 2
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 Internat
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 261765
EOR
F002 518
F010 3.7
F004 2
F005 RL
F006 This robust summary was given a reliability rating of 2 because the data
* were not retrieved and reviewed for quality. The data were reported by
* the Japanese National Institute of Technology and Evaluation and are
* believed to be reliable.
F007 This robust summary was given a reliability rating of 2 because the data
* were not retrieved and reviewed for quality. The data were reported by
* the Japanese National Institute of Technology and Evaluation and are
* believed to be reliable.
F020 261764
EOR
F002 518
F010 3.7
F004 2
F005 RS
F006 BCF for test:
**
** 100 ug/l = 12 to 38
** 10 ug/l = 23 to 45

**
** Low potential to bioconcentrate.
F007 BCF for test:
**
** 100 ug/l = 12 to 38
** 10 ug/l = 23 to 45
**
** Low potential to bioconcentrate.
F020 261763
EOR
F002 518
F010 3.7
F004 2
F005 TS
F006 CAS No. 110-83-8; cyclohexene; purity is unknown
F007 CAS No. 110-83-8; cyclohexene; purity is unknown
F020 261761
EOR
F002 518
F010 4.1
F004 1
F005 ME
F006 ECOSAR version 0.99h, U.S. 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 h
F007 ECOSAR version 0.99h, U.S. 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 261770
EOR
F002 518
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 261777
EOR
F002 518
F010 4.1
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 261772
EOR
F002 518
F010 4.1
F004 1
F005 RS
F006
** Calculated 96-hr LC50 for fish = 7.6 mg/L
F007
** Calculated 96-hr LC50 for fish = 7.6 mg/L
F020 261771
EOR
F002 518
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 EPIWIN computer model (2). KOWWIN also has a database

* of experimental Kow values (EXPKOW.DB).
**
** The ECOSAR program was run using cyclohexene with a Kow of 2.86.
**
** 1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for
* estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.
**
** 2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer
* program EPIWIN. 1999. Estimation Program Interface for Windows, version
* 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
F020 261773
EOR
F002 518
F010 4.1
F004 1
F005 TS
F006 CAS No. 110-83-8; cyclohexene; purity is unknown
F007 CAS No. 110-83-8; cyclohexene; purity is unknown
F020 261766
EOR
F002 518
F010 4.1
F004 2
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 Internat
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 261776
EOR
F002 518
F010 4.1
F004 2
F005 RL
F006 This robust summary was given a reliability rating of 2 because the data
* were not retrieved and evaluated for quality, however, the data were
* reported by a reliable source.
F007 This robust summary was given a reliability rating of 2 because the data
* were not retrieved and evaluated for quality, however, the data were
* reported by a reliable source.
F020 261775
EOR
F002 518
F010 4.1
F004 2
F005 RM
F006 Study reported by the Japanese National Institute of Technology and

* Evaluation on their website. No other information regarding the study
* was reported. Remarks were available, but only in Japanese.
F007 Study reported by the Japanese National Institute of Technology and
* Evaluation on their website. No other information regarding the study
* was reported. Remarks were available, but only in Japanese.
F020 261774
EOR
F002 518
F010 4.1
F004 2
F005 TS
F006 CAS No. 110-83-8; cyclohexene; purity is unknown
F007 CAS No. 110-83-8; cyclohexene; purity is unknown
F020 261767
EOR
F002 518
F010 4.1
F004 3
F005 RE
F006 Morrow, J., Gritz, R. and Kirton, M. (1975). Effects of Some Components
* of Crude Oil on Young Coho Salmon. Copeia. No. 2: 326-331
F007 Morrow, J., Gritz, R. and Kirton, M. (1975). Effects of Some Components
* of Crude Oil on Young Coho Salmon. Copeia. No. 2: 326-331
F020 261787
EOR
F002 518
F010 4.1
F004 3
F005 RL
F006 This robust summary was given a reliability rating of 3 because the study
* was performed in open test vessels with full aeration. Given the
* volatility of the test substance, an open vessel is not an appropriate
* test design.
F007 This robust summary was given a reliability rating of 3 because the study
* was performed in open test vessels with full aeration. Given the
* volatility of the test substance, an open vessel is not an appropriate
* test design.
F020 261786
EOR
F002 518
F010 4.1
F004 3
F005 RM
F006 The study was performed in open vessels with full aeration in 30 ppt
* artificial seawater made with Instant Ocean brand seasalts. Fish were
* not fed during the experiment. Test tanks were 95 liter tanks containing
* 75 liters of water. The t
F007 The study was performed in open vessels with full aeration in 30 ppt
* artificial seawater made with Instant Ocean brand seasalts. Fish were
* not fed during the experiment. Test tanks were 95 liter tanks containing
* 75 liters of water. The test substance was added to the test tank via a
* syringe to simulate an oil spill.

**
** Loading of the test tank was adjusted to provide less than 1g of fish per
* liter of seawater. Cyclohexene was tested at 100 and 50 ppm. Fish were
* observed to "spasm" at both concentrations of cyclohexene upon additiona
* of the test substance to the water. Fish returned to "normal" after a
* short time interval (2 to 4 hours). No significant mortality was noted
* in the test.
F020 261785
EOR
F002 518
F010 4.1
F004 3
F005 TS
F006 CAS No. 110-83-8; cyclohexene; purity is unknown
F007 CAS No. 110-83-8; cyclohexene; purity is unknown
F020 261784
EOR
F002 518
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 261778
EOR
F002 518
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 261781
EOR
F002 518
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 EPIWIN computer model (2). KOWWIN also has a database
* of experimental Kow values (EXPKOW.DB).
**
** The ECOSAR program was run using cyclohexene with a Kow of 2.86.
**
** 1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for
* estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.
**
** 2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer
* program EPIWIN. 1999. Estimation Program Interface for Windows, version
* 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
F020 261780
EOR
F002 518
F010 4.2
F004 1
F005 TS
F006 CAS No. 110-83-8; cyclohexene; purity is unknown
F007 CAS No. 110-83-8; cyclohexene; purity is unknown
F020 261768
EOR
F002 518
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 261779
EOR
F002 518
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 261782
EOR
F002 518
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 EPIWIN computer model (2). KOWWIN also has a database
* of experimental Kow values (EXPKOW.DB).
**
** The ECOSAR program was run using cyclohexene with a Kow of 2.86.
**
** 1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for
* estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.
**
** 2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer
* program EPIWIN. 1999. Estimation Program Interface for Windows, version
* 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
F020 261783
EOR
F002 518
F010 4.3
F004 1
F005 TS
F006 CAS No. 110-83-8; cyclohexene; purity is unknown
F007 CAS No. 110-83-8; cyclohexene; purity is unknown
F020 261769
EOR
F002 518
F010 5.1.1
F004 1
F005 RE
F006 MHLW (Ministry of Health, Labour and Welfare), Japan (2002) Toxicity
* Testing Reports of Environmental Chemicals, 9, 233-234.
F007 MHLW (Ministry of Health, Labour and Welfare), Japan (2002) Toxicity
* Testing Reports of Environmental Chemicals, 9, 233-234.
F020 260275
EOR
F002 518
F010 5.1.1
F004 1
F005 RM
F006 Doses were 0, 500, 1000, and 2000 mg/kg bw for both sexes.
F007 Doses were 0, 500, 1000, and 2000 mg/kg bw for both sexes.
F020 260271
EOR
F002 518
F010 5.1.1
F004 1
F005 RS
F006 LD50 value was greater than 1,000 mg/kg bw.
** Each 3 of 5 animals of male and female rats at 2,000 mg/kg bw showed
* abnormal gait, adoption of a prone position, salivation, piloerection and

* tremor, and then died within 3 days after dosing. Hyp
F007 LD50 value was greater than 1,000 mg/kg bw.
** Each 3 of 5 animals of male and female rats at 2,000 mg/kg bw showed
* abnormal gait, adoption of a prone position, salivation, piloerection and
* tremor, and then died within 3 days after dosing. Hypoactivity was
* observed in all male and female rats given the test substance.
* Lacrimation was also observed in both sexes just after dosing at 1,000
* mg/kg bw and more. Necropsy of the dead animals revealed pulmonary
* congestion.
**
** Mortality:

**	Dose(mg/kgbw)		0	500	1000	2000
**	No.of animals		5	5	5	5
**	No.of d	0	0	0	3	
**	Female		0	0	0	3

F020 260272
EOR
F002 518
F010 5.1.1
F004 1
F005 SO
F006 Research Institute for Animal Science in Biochemistry and Toxicology
* Sagamihara Kanagawa
F007 Research Institute for Animal Science in Biochemistry and Toxicology
* Sagamihara Kanagawa
F020 260273
EOR
F002 518
F010 5.1.1
F004 1
F005 TS
F006 Purity: 98.6%
F007 Purity: 98.6%
F020 260274
EOR
F002 518
F010 5.1.2
F004 1
F005 RE
F006 NTIS (National Technical Information Service): OTS0555329
F007 NTIS (National Technical Information Service): OTS0555329
F020 260276
EOR
F002 518
F010 5.1.2
F004 1
F005 RM
F006 Value: > 6370 ppm (> 21388 mg/m3)
F007 Value: > 6370 ppm (> 21388 mg/m3)
F020 260347
EOR
F002 518

F010 5.1.2
F004 1
F005 RS
F006 Toxic effects: Tremor and ataxia.
F007 Toxic effects: Tremor and ataxia.
F020 260277
EOR
F002 518
F010 5.1.2
F004 1
F005 SO
F006 Research Institute for Animal Science in Biochemistry and Toxicology
* Sagamihara Kanagawa
F007 Research Institute for Animal Science in Biochemistry and Toxicology
* Sagamihara Kanagawa
F020 260278
EOR
F002 518
F010 5.1.3
F004 1
F005 RE
F006 NTIS (National Technical Information Service): OTS0556686
F007 NTIS (National Technical Information Service): OTS0556686
F020 260281
EOR
F002 518
F010 5.1.3
F004 1
F005 RS
F006 Details of toxic effects were not reported other than lethal dose value.
F007 Details of toxic effects were not reported other than lethal dose value.
F020 260279
EOR
F002 518
F010 5.1.3
F004 1
F005 SO
F006 Research Institute for Animal Science in Biochemistry and Toxicology
* Sagamihara Kanagawa
F007 Research Institute for Animal Science in Biochemistry and Toxicology
* Sagamihara Kanagawa
F020 260280
EOR
F002 518
F010 5.4
F004 1
F005 CL
F006 Increase in total bile acid noted in females of 50 mg/kg bw was not
* considered as an adverse effect because of no accompanying changes.
** Therefore, based on salivation observed at 150 mg/kg bw, the NOAEL for
* repeated dose toxicity was consid
F007 Increase in total bile acid noted in females of 50 mg/kg bw was not

* considered as an adverse effect because of no accompanying changes.
** Therefore, based on salivation observed at 150 mg/kg bw, the NOAEL for
* repeated dose toxicity was considered to be 50 mg/kg bw/day.
F020 260287
EOR
F002 518
F010 5.4
F004 1
F005 RE
F006 MHLW (Ministry of Health, Labour and Welfare), Japan (2002) Toxicity
* Testing Reports of Environmental Chemicals, 9, 235-243.
F007 MHLW (Ministry of Health, Labour and Welfare), Japan (2002) Toxicity
* Testing Reports of Environmental Chemicals, 9, 235-243.
F020 260282
EOR
F002 518
F010 5.4
F004 1
F005 RM
F006 This study was conducted to examine both repeated dose toxicity and
* reproductive/developmental toxicity as an OECD screening combined study
* (Test guideline: 422).
** Study design:
** Vehicle: Corn oil
** Clinical observation performed and frequency:
F007 This study was conducted to examine both repeated dose toxicity and
* reproductive/developmental toxicity as an OECD screening combined study
* (Test guideline: 422).
** Study design:
** Vehicle: Corn oil
** Clinical observation performed and frequency: General condition was
* observed once a day, body weights were determined at days 1 (before
* dosing),8, 15, 22, 29, 36, 43 and 49 of treatment for males and at days
* 1, 8 and 15 of treatment and at days 0, 7, 14, and 20 of gestation period
* and at days 0 and 4 of lactation period and at autopsy for females, food
* consumption was determined at days 1, 8, 15, 22, 29, 36, 43 and 48 of
* treatment for males and at days 1,8 and 15 of treatment and at days 0, 7,
* 14 and 20 of gestation period and at days 0 and 4 of lactation for
* females, but food consumption were not determined during mating period
* for males and females.
** For 5 males per group, urinalysis was carried out at 43-48 days of
* administration period. For all males and all females after childbirth,
* hematology and biochemistry were carried out at time of necropsy after 49
* days for males and at 5 days after delivery for females. Organs examined
* at necropsy.
** Organ weight: Brain, liver, kidney, spleen, adrenal, thymus, testis and
* epididymis
** Microscopic examination: Brain, pituitary, thymus, thyroid, parathyroid,
* adrenal, spleen, heart, thoracic aorta, tongue, esophagus, stomach,
* liver, pancreas, duodenum, jejunum, ileum, cecum, colon, rectum, larynx,
* trachea, lung, kidney, urinary bladder, testis, epididymis, prostate,
* seminal

** vesicle, ovary, uterus, vagina, eye, harderian gland, mammary gland,
* skin, sternum, femur, spinal cord, skeletal muscle, mesentery lymph node,
* mandibular lymph node, submandibular gland, sublingual gland, parotid
* gland, ischiadic nerve, bone marrow, Statistical methods: Dunnett's test
* for continuous data and Steel test for quantal data.
F020 260283
EOR
F002 518
F010 5.4
F004 1
F005 RS
F006 Mortality: There was no mortality related to the test substance
* treatment. Clinical signs: Salivation was apparent in three animals of
* 150 mg/kg bw group and in twelve animals of 500 mg/kg bw group for males
* and in two animals of 150 mg/kg
F007 Mortality: There was no mortality related to the test substance
* treatment. Clinical signs: Salivation was apparent in three animals of
* 150 mg/kg bw group and in twelve animals of 500 mg/kg bw group for males
* and in two animals of 150 mg/kg bw group and twelve animals of 500 mg/kg
* bw group for females. Although the grades of salivation were not
* reported, the sign was observed for about 5 minutes after dosing at 150
* mg/kg bw, and for 30 minutes to 5 hours after dosing at 500 mg/kg bw
* during treatment period. In addition, lacrimation was observed in two
* animals of 500 mg/kg bw group for males and in one animal each of 150 and
* 500 mg/kg bw groups for females. The onsets and grades of lacrimation
* were not reported.
** Body weight: No statistically significant changes for males and females.
** Food consumption: No effects for males and females.
** Urinalysis: No statistically significant changes.
** Hematology: No effects for males and females
** Blood biochemistry: Males: Decreases in triglyceride in 150 and 500 mg/kg
* bw groups, increases in total bilirubin in 500 mg/kg bw group, and total
* bile acid in 150 and 500 mg/kg bw.
**

**	Dose (mg/kg bw)		0	50	150	500		
**	No.of animals			12	11	12	12	
**	Triglyce	39.2	6.8	27.7	22.5			
**		SD			22.4	18.8	16.7	7.7
**	T.bilirul	0.03	0.04	0.05	0.05*			
**		SD			0.01	0.01	0.01	0.01
**	T.bile a	18.8	20.8	39.9*	32.6			
**		SD			15	16.6	21	25.5

** Note: *, P<0.05
**
** Females: Increase in total bile acid in 50, 150, and 500 mg/kg bw.
**

** T.bile a

** Necropsy and histopathology: No adverse effects for males and females
** Organ weights: Males: Increase in a relative kidney weight in 500 mg/kg
* bw group.
**
** Dose (mg/kg bw) 0 50 150 500
** No.of animals 12 11 12 12
** Kidney 3.21 3.09 3.2 3.31
** SD 0.33 0.27 0.27 0.27
** Relative (g%) Mea 0.652 0.619 0.667 0.705*
** SD 0.057 0.031 0.059 0.053
** Note: *, p<0.05
**
** Females: No statistically significant changes.
**
** Histopathology: No changes related to test substance.
F020 260284
EOR
F002 518
F010 5.4
F004 1
F005 SO
F006 Research Institute for Animal Science in Biochemistry and Toxicology
* Sagamihara Kanagawa
F007 Research Institute for Animal Science in Biochemistry and Toxicology
* Sagamihara Kanagawa
F020 260285
EOR
F002 518
F010 5.4
F004 1
F005 TS
F006 Purity: 98.6%
F007 Purity: 98.6%
F020 260286
EOR
F002 518
F010 5.5
F004 1
F005 RE
F006 MHLW (Ministry of Health, Labour and Welfare), Japan (2002) Toxicity
* Testing Reports of Environmental Chemicals, 9, 251-254.
F007 MHLW (Ministry of Health, Labour and Welfare), Japan (2002) Toxicity
* Testing Reports of Environmental Chemicals, 9, 251-254.
F020 260292
EOR
F002 518
F010 5.5
F004 1
F005 RM
F006 Procedures: Pre-incubation method
** Solvent: Ethanol
** Dosage of each strain with or without S9

** -S9 mix: 0, 19.5, 39.1, 78.1, 156, 313, 625, 1250 ug/plate
** (TA100, TA1535, TA98, TA1537); 0, 78.1, 156, 313, 625, 1250, 2500, 5000
* ug/plate (WP2 uvr
F007 Procedures: Pre-incubation method
** Solvent: Ethanol
** Dosage of each strain with or without S9
** -S9 mix: 0, 19.5, 39.1, 78.1, 156, 313, 625, 1250 ug/plate
** (TA100, TA1535, TA98, TA1537); 0, 78.1, 156, 313, 625, 1250, 2500, 5000
* ug/plate (WP2 uvrA)
** +S9 mix: 0, 19.5, 39.1, 78.1, 156, 313, 625, 1250 ug/plate (all strain)
** *Maximum concentration was established based on the result of the
* preliminary test up to 5000 ug/plate. In this test, the growth inhibition
* was observed at 1250 ug/plate and more with and without S9 mix in
* Salmonella typhimurium TA100, TA98, TA1535, TA1537 and with S9 mix in
* Escherichia coli WP2 uvrA.
** Positive control: without S9 mix:
** 2-(2-furyl)-3-(5-nitro-2-furyl)acrylamide (TA100, TA98, WP2 uvrA), Sodium
* azide (TA 1535),
* 2-methoxy-6-chloro-9-[3-(2-chloroethyl)-aminopropylamino]acriine 2HCl
** with S9 mix: Benzo[a]pyrene (TA100, TA98), 2-aminoanthracene (TA1535, WP2
* uvrA, TA1537)
** S9: Rat liver, induced with phenobarbital and 5,6-benzoflavone
** Plates/test: 3
F020 260288
EOR
F002 518
F010 5.5
F004 1
F005 RS
F006 There were no precipitations in any test concentration.
** Cytotoxic concentration: Growth inhibition was observed at 625 ug/plate
* or more with or without S9 mix in Salmonella typhimurium TA100, TA1535,
* TA98, TA1537, and at 1250 ug/plate or mo
F007 There were no precipitations in any test concentration.
** Cytotoxic concentration: Growth inhibition was observed at 625 ug/plate
* or more with or without S9 mix in Salmonella typhimurium TA100, TA1535,
* TA98, TA1537, and at 1250 ug/plate or more with S9 in Escherichia coli
* WP2 uvrA.
** Genotoxic effects:
** With metabolic activation: negative
** Without metabolic activation: negative
F020 260289
EOR
F002 518
F010 5.5
F004 1
F005 SO
F006 Research Institute for Animal Science in Biochemistry and Toxicology
* Sagamihara Kanagawa
F007 Research Institute for Animal Science in Biochemistry and Toxicology
* Sagamihara Kanagawa
F020 260290

EOR
F002 518
F010 5.5
F004 1
F005 TS
F006 Purity: 98.63%
F007 Purity: 98.63%
F020 260291
EOR
F002 518
F010 5.5
F004 2
F005 RE
F006 MHLW (Ministry of Health, Labour and Welfare), Japan (2002) Toxicity
* Testing Reports of Environmental Chemicals, 9, 255-259.
F007 MHLW (Ministry of Health, Labour and Welfare), Japan (2002) Toxicity
* Testing Reports of Environmental Chemicals, 9, 255-259.
F020 260293
EOR
F002 518
F010 5.5
F004 2
F005 RM
F006 Solvent: Ethanol
** S9: Rat liver, induced with phenobarbital and 5,6-benzoflavone
** Plates/test: 2
** The maximum concentration was established, based on the growth inhibition
* test. In this test, 50% growth inhibition was observed between 250 and
F007 Solvent: Ethanol
** S9: Rat liver, induced with phenobarbital and 5,6-benzoflavone
** Plates/test: 2
** The maximum concentration was established, based on the growth inhibition
* test. In this test, 50% growth inhibition was observed between 250 and
* 300 ug/mL for short-term treatment and continuous treatment with or
* without S9.
F020 260294
EOR
F002 518
F010 5.5
F004 2
F005 RS
F006 No increase in chromosomal aberrations was observed after short-term or
* continuous treatment with or without S9 mix.
** Cell toxicity was observed at 400 ug/mL after continuous treatments for
* 24 and 48 hrs.
F007 No increase in chromosomal aberrations was observed after short-term or
* continuous treatment with or without S9 mix.
** Cell toxicity was observed at 400 ug/mL after continuous treatments for
* 24 and 48 hrs.
F020 260295
EOR
F002 518

F010 5.5
F004 2
F005 SO
F006 Research Institute for Animal Science in Biochemistry and Toxicology
* Sagamihara Kanagawa
F007 Research Institute for Animal Science in Biochemistry and Toxicology
* Sagamihara Kanagawa
F020 260296
EOR
F002 518
F010 5.5
F004 2
F005 TS
F006 Purity: 98.63%
F007 Purity: 98.63%
F020 260297
EOR
F002 518
F010 5.8.1
F004 1
F005 RE
F006 MHLW (Ministry of Health, Labour and Welfare), Japan (2002) Toxicity
* Testing Reports of Environmental Chemicals, 9, 235-243.
F007 MHLW (Ministry of Health, Labour and Welfare), Japan (2002) Toxicity
* Testing Reports of Environmental Chemicals, 9, 235-243.
F020 260352
EOR
F002 518
F010 5.8.1
F004 1
F005 RM
F006 This study was conducted to examine both repeated dose toxicity and
* reproductive/developmental toxicity as an OECD screening combined study
* (Test guideline: 422).
** Study design:
** Vehicle: Corn oil
** Clinical observation performed and frequency:
F007 This study was conducted to examine both repeated dose toxicity and
* reproductive/developmental toxicity as an OECD screening combined study
* (Test guideline: 422).
** Study design:
** Vehicle: Corn oil
** Clinical observation performed and frequency: General condition was
* observed once a day, body weights were determined at days 1 (before
* dosing), 8, 15, 22, 29, 36, 43 and 49 of treatment for males and at days
* 1, 8 and 15 of treatment and at days 0, 7, 14, and 20 of gestation period
* and at days 0 and 4 of lactation period and at autopsy for females, food
* consumption was determined at days 1, 8, 15, 22, 29, 36, 43 and 48 of
* treatment for males and at days 1,8 and 15 of treatment and at days 0, 7,
* 14 and 20 of gestation period and at days 0 and 4 of lactation for
* females, but food consumption were not determined during mating period
** for males and females.

** For 5 males per group, urinalysis was carried out at 43-48 days of
* administration period. For all males and all females after childbirth per
* group, hematology and biochemistry were carried out at time of necropsy
* after 49 days for males and at 5 days after delivery for females. Organs
* examined at necropsy.
** Organ weight: Brain, liver, kidney, spleen, adrenal, thymus, testis and
* epididymis
** Microscopic examination: Brain, pituitary, thymus, thyroid, parathyroid,
* adrenal, spleen, heart, thoracic aorta, tongue, esophagus, stomach,
* liver, pancreas, duodenum, jejunum, ileum, cecum, colon, rectum, larynx,
* trachea, lung, kidney, urinary bladder, testis, epididymis, prostate,
* seminal vesicle, ovary, uterus, vagina, eye, harderian gland, mammary
* gland, skin, sternum, femur, spinal cord, skeletal muscle, mesentery
* lymph node, mandibular lymph node, submandibular gland, sublingual gland,
* parotid gland, ischiadic nerve, bone marrow.
** Reproductive and developmental parameters: No.of pairs with successful
* copulation, No. of pregnant females, copulation index (No. of pairs with
* successful copulation/No. of pairs mated x 100), fertility index (No. of
* pregnant animals/No.of animals with successful copulation x 100), estrous
* cycle, No. of dams delivered live pups, duration of gestation, No. of
* total corpora lutea, No. of total implants, No. of total pups born, No.
* of total live pups born, sex ratio, No. of total dead pups, No. of total
* cannibalism, gestation index (No. of females with live pups/No. of
* pregnant females x 100), implantation index (No. of implants/No.of
* corpora lutea x 100), delivery index (No. of pups born/No. of implants x
* 100), live birth index (No. of live pups born/No. of pups born x 100),
* and viability index on day 4 (No. of live pups on day 4 after birth/No.
* of live pups born x 100). Statistical methods: Dunnett's test for
* continuous data and Steel test for quantal data.
F020 260348
EOR
F002 518
F010 5.8.1
F004 1
F005 RS
F006 Mortality: There was no mortality related to the test substance treatment.
** Clinical signs: Salivation was apparent in three animals of 150 mg/kg bw
* group and in twelve animals of 500 mg/kg bw group for males and in two
* animals of 150 mg/kg
F007 Mortality: There was no mortality related to the test substance treatment.
** Clinical signs: Salivation was apparent in three animals of 150 mg/kg bw
* group and in twelve animals of 500 mg/kg bw group for males and in two
* animals of 150 mg/kg bw group and twelve animals of 500 mg/kg bw group
* for females. Although the grades of salivation were not reported, the
* sign was observed for about 5 minutes after dosing at 150 mg/kg bw, and
* for 30 minutes to 5 hours after dosing at 500 mg/kg bw during treatment
* period. In addition, lacrimation was observed in two animals of 500 mg/kg
* bw group for males and in one animal each of 150 and 500 mg/kg bw groups
* for females. The onsets and grades of lacrimation were not reported.
** Body weight: No statistically significant changes for males and females.
** Food consumption: No effects for males and females.
** Urinalysis: No statistically significant changes.

** Hematology: No effects for males and females
** Blood biochemistry:
** Males: Decreases in triglyceride in 150 and 500 mg/kg bw groups,
* increases in total bilirubin in 500 mg/kg bw group, and total bile acid
* in 150 and 500 mg/kg bw.
** Females: Increase in total bile acid in 50, 150, and 500 mg/kg bw.
** Necropsy and histopathology: No adverse effects for males and females.
** Organ weights:
** Males: Increase in a relative kidney weight in 500 mg/kg bw group.
** Females: No statistically changes.
**
** Histopathology: No changes related to test substance.
** Reproductive and developmental parameters: No effects observed on
* reproductive performance in males and females given each dose, and
* developmental performance of the newborns.
**

** Dose(mg/kg bw)		0	50	150	500	
** No. of pairs mated	12	12	12	12		
** No. of pairs copula	12	11	12	12		
** No. of pregnant fer	11	10	10	10		
** Copulation index (%	100	91.7	100	100		
** Fertility index (%)	91.7	90.9	83.3	83.3		
** No. of dams obser	11	10	10	10		
** No. of dams delivered						
** live pups		11	10	10	10	
** Duration of gestation:						
** Mean			22.5	22.2	22.3	22.5
** SD			0.5	0.4	0.5	0.5
** No. of total corpora lutea:						
** Mean			19.2	17.4	18.4	20.1
** SD			2.6	3.3	3.2	3.8
** No. of total implants:						
** Mean			13.7	14.4	14.3	14.3
** SD			3	1.6	1.5	1.6
** No. of total pups born:						
** Mean			12.8	13.4	13.5	12.5
** SD			3.5	1.6	2.1	2.2
** Sex rat Mean		0.8	1.32	1.14	0.81	
** SD			0.23	0.68	1.6	0.56
** No. of total live pups on day 4						
** Male: Mean			5.5	6.9	6.7	5
** SD			2.2	1.9	2.4	2
** Female: Mean		6.8	6.2	6.7	7.2	
** SD			2.8	1.9	2.4	2
** No. of total dead pups:						

** Gestation index (%

**		Mean		93.2	93.8	97.3	90
**		SD		11.9	6.1	4.7	10.3
**	Live birth index (%):						
**		Mean		98	99.3	96.9	97
**		SD		4.7	2.3	9.7	9.5
**	Viability index day 4						
**	Male:	Mean		90.9	95.3	100	96.7
**		SD		30.2	10	0	10.5
**	Female:	Mean	88.6	100	98.3	98.3	
**		SD		29.8	0	5.3	5.3

F020 260349
EOR
F002 518
F010 5.8.1
F004 1
F005 SO
F006 Research Institute for Animal Science in Biochemistry and Toxicology
* Sagamihara Kanagawa
F007 Research Institute for Animal Science in Biochemistry and Toxicology
* Sagamihara Kanagawa
F020 260350
EOR
F002 518
F010 5.8.1
F004 1
F005 TS
F006 Purity: 98.6%
F007 Purity: 98.6%
F020 260351
EOR
F002 518
F010 5.8.2
F004 1
F005 RE
F006 MHLW (Ministry of Health, Labour and Welfare), Japan (2002) Toxicity
* Testing Reports of Environmental Chemicals, 9, 235-243.
F007 MHLW (Ministry of Health, Labour and Welfare), Japan (2002) Toxicity
* Testing Reports of Environmental Chemicals, 9, 235-243.
F020 260303
EOR
F002 518
F010 5.8.2
F004 1
F005 RM
F006 This study was conducted to examine both repeated dose toxicity and
* reproductive/developmental toxicity as an OECD screening combined study
* (Test guideline: 422).
** Study design:
** Vehicle: Corn oil
** Clinical observation performed and frequency:
F007 This study was conducted to examine both repeated dose toxicity and
* reproductive/developmental toxicity as an OECD screening combined study

* (Test guideline: 422).
** Study design:
** Vehicle: Corn oil
** Clinical observation performed and frequency: General condition was
* observed once a day, body weights were determined at days 1 (before
* dosing), 8, 15, 22, 29, 36, 43 and 49 of treatment for males and at days
* 1, 8 and 15 of treatment and at days 0, 7, 14, and 20 of gestation period
* and at days 0 and 4 of lactation period and at autopsy for females, food
* consumption was determined at days 1, 8, 15, 22, 29, 36, 43 and 48 of
* treatment for males and at days 1,8 and 15 of treatment and at days 0, 7,
* 14 and 20 of gestation period and at days 0 and 4 of lactation for
* females, but food consumption were not determined during mating period
** for males and females.
** For 5 males per group, urinalysis was carried out at 43-48 days of
* administration period. For all males and all females after childbirth per
* group, hematology and biochemistry were carried out at time of necropsy
* after 49 days for males and at 5 days after delivery for females. Organs
* examined at necropsy.
** Organ weight: Brain, liver, kidney, spleen, adrenal, thymus, testis and
* epididymis
** Microscopic examination: Brain, pituitary, thymus, thyroid, parathyroid,
* adrenal, spleen, heart, thoracic aorta, tongue, esophagus, stomach,
* liver, pancreas, duodenum, jejunum, ileum, cecum, colon, rectum, larynx,
* trachea, lung, kidney, urinary bladder, testis, epididymis, prostate,
* seminal vesicle, ovary, uterus, vagina, eye, harderian gland, mammary
* gland, skin, sternum, femur, spinal cord, skeletal muscle, mesentery
* lymph node, mandibular lymph node, submandibular gland, sublingual gland,
* parotid gland, ischiadic nerve, bone marrow.
** Reproductive and developmental parameters: No.of pairs with successful
* copulation, No. of pregnant females, copulation index (No. of pairs with
* successful copulation/No. of pairs mated x 100), fertility index (No. of
* pregnant animals/No.of animals with successful copulation x 100), estrous
* cycle, No. of dams delivered live pups, duration of gestation, No. of
* total corpora lutea, No. of total implants, No. of total pups born, No.
* of total live pups born, sex ratio, No. of total dead pups, No. of total
* cannibalism, gestation index (No. of females with live pups/No. of
* pregnant females x 100), implantation index (No. of implants/No.of
* corpora lutea x 100), delivery index (No. of pups born/No. of implants x
* 100), live birth index (No. of live pups born/No. of pups born x 100),
* and viability index on day 4 (No. of live pups on day 4 after birth/No.
* of live pups born x 100). Statistical methods: Dunnett's test for
* continuous data and Steel test for quantal data.
F020 260304
EOR
F002 518
F010 5.8.2
F004 1
F005 RS
F006 There was no mortality related to the test substance treatment.
* Salivation was apparent in three animals of 150 mg/kg bw group and in
* twelve animals of 500 mg/kg bw group for males and in two animals of 150
* mg/kg bw group and twelve animals

F007 There was no mortality related to the test substance treatment.
* Salivation was apparent in three animals of 150 mg/kg bw group and in
* twelve animals of 500 mg/kg bw group for males and in two animals of 150
* mg/kg bw group and twelve animals of 500 mg/kg bw group for females.
* Although the grades of salivation were not reported, the sign was
* observed for about 5 minutes after dosing at 150 mg/kg bw, and for 30
* minutes to 5 hours after dosing at 500 mg/kg bw during treatment period.
* In addition, lacrimation was observed in two animals of 500 mg/kg bw
* group for males and in one animal each of 150 and 500 mg/kg bw groups for
* females. The onsets and grades of lacrimation were not reported.
**
** There were no statistically significant changes in body weight, food
* consumption, urinalysis and hematology for males and females.
**
** Blood biochemistry:
** Males: Decreases in triglyceride in 150 and 500 mg/kg bw groups,
* increases in total bilirubin in 500 mg/kg bw group, and total bile acid
* in 150 and 500 mg/kg bw.
** Females: Increase in total bile acid in 50, 150, and 500 mg/kg bw.
** Necropsy and histopathology: No adverse effects for males and females.
** Organ weights:
** Males: Increase in a relative kidney weight in 500 mg/kg bw group.
** Females: No statistical changes.
**
** Histopathology: No changes related to test substance.
** Reproductive and developmental parameters: No effects observed on
* reproductive performance in males and females given each dose, and
* developmental performance of the newborns.
**

**	Dose(mg/kg bw)		0	50	150	500
**	No. of total pups born:					
**		Mean		12.8	13.4	13.5	12.5
**		SD		3.5	1.6	2.1	2.2
**	Sex rat Mean		0.8	1.32	1.14	0.81	
**		SD		0.23	0.68	1.6	0.56
**	No. of total live pups on day 4					
**	Male:	Mean		5.5	6.9	6.7	5
**		SD		2.2	1.9	2.4	2
**	Female:	Mean	6.8	6.2	6.7	7.2	
**		SD		2.8	1.9	2.4	2
**	No. of total dead pups:					
**		Mean		0.3	0.1	0.1	0
**		SD		0.6	0.3	0.3	0
**	Viability index day 4					
**	Male:	Mean		90.9	95.3	100	96.7
**		SD		30.2	10	0	10.5
**	Female:	Mean	88.6	100	98.3	98.3	
**		SD		29.8	0	5.3	5.3

F020 260305
EOR
F002 518
F010 5.8.2

F004 1
F005 SO
F006 Research Institute for Animal Science in Biochemistry and Toxicology
* Sagamihara Kanagawa
F007 Research Institute for Animal Science in Biochemistry and Toxicology
* Sagamihara Kanagawa
F020 260306
EOR
F002 518
F010 5.8.2
F004 1
F005 TS
F006 Purity: 98.6%
F007 Purity: 98.6%
F020 260307
EOB
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X

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C International Uniform ChemicaL Information Database
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C Column 6-80: Blockname  / Fieldvalue
C Date      : 01-OCT-2007 12:59:33
C Company   : ExxonMobil Biomedical Sciences Inc.  08801-3059  Annadale, New Je
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V   IUCLID-Export V4.00
C
CS  ISO-Latin 1
C
NL  GBR
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F001 994-05-8
F002 Y26-001
EOB
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B006 SUBST_IDENT_TAB
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F003 Y27-030
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F001 994-05-8
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F003 Y27-003
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F001 994-05-8
F009 N
F005 12032693
F006 28-07-2006
F007 12032693
F008 28-07-2006
F003 09-10-2006
F101 U.S. EPA - HPV Challenge Program
F102 A35-02
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B004 COMPANY_TAB
F001 12032693
F003 ExxonMobil Biomedical Sciences Inc.
F004 1545 Route 22 East
F005 Annadale, New Jersey
F006 08801-3059
F008 A31-024
EOB
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B052 DS_COMPONENT_JOIN_TAB
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F005 1
F006 28-07-2006
F007 28-07-2006
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F005 1
F006 31-07-2006
F007 31-07-2006
EOR
F001 482
F002 0
F003 2.2
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F005 1
F006 31-07-2006
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F001 482
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F005 1
F006 31-07-2006
F007 31-07-2006
EOR
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F007 31-07-2006
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F007 31-07-2006
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F001 482

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F001 482
F002 0
F003 5.5
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F006 09-10-2006
F007 31-07-2006
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F001 482
F002 0
F003 5.5
F004 2
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F001 482
F002 0
F003 5.6
F004 1

F005 1
F006 09-10-2006
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F001 482
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F007 31-07-2006
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F001 482
F002 0
F003 5.8.2
F004 1
F005 1
F006 09-10-2006
F007 31-07-2006
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F001 482
F002 0
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F004 2
F005 2
F006 09-10-2006
F007 31-07-2006
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B053 DS_REC_MARK_TAB
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F004 A37-009
EOR
F001 482
F002 2.2
F003 1
F004 A37-009
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F002 2.6.1

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F004 A37-009
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F004 A37-009
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F004 A37-009
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B051 DS_COMPONENT_TAB
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F003 994-05-8
F012 N
F010 28-07-2006
F004 12032693
F005 28-07-2006
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F006 12032693
F007 28-07-2006
F008 U.S. EPA - HPV Challenge Program
F009 A35-02
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B101 GI_GENERAL_INFORM_TAB
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F004 CLGETTS
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F010 A04-04
F011 A19-02
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B201 PC_MELTING_TAB
F001 482
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F003 31-07-2006
F004 CLGETTS1
F016 1
F007 A02-03
F008 -81.2
F012 P01-03:  calculated
F014 A03-02
F020 A01-03: tert-amyl methyl ether (TAME); (CAS #994-05-8)
**   Melting Point is calculated by the MPBPWIN, version 1.41, a subroutine of
*    the computer program EPI SuiteTM, version 3.012, (2000) which is based on
*    the average result of the meth
EOB
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B202 PC_BOILING_TAB
F001 482
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F004 CLGETTS1
F016 A36-003
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F013 P03-03:  not specified
F015 A03-02
F018 A01-03: tert-amyl methyl ether (TAME); (CAS #994-05-8)
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B203 PC_DENSITY_TAB
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F016 A36-003
F017 1
F007 P05-02
F008 A02-03
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F013 P04-03:  not specified
F015 A03-02
F018 A01-03: tert-amyl methyl ether (TAME); (CAS #994-05-8)
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B204 PC_VAPOUR_TAB
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F007 A02-03
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F014 A03-02
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F003 31-07-2006
F004 CLGETTS1
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F010 P02-01
F011 25
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F014 A03-02
F018 A01-03: tert-amyl methyl ether (TAME); (CAS #994-05-8)
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F001 482
F002 3
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F004 CLGETTS1
F015 A36-003
F016 3
F007 A02-03
F008 210
F010 P02-01
F011 37.8
F012 P06-04
F014 A03-02
F018 A01-03: tert-amyl methyl ether (TAME); (CAS #994-05-8)
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B205 PC_PARTITION_TAB
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F004 CLGETTS1
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F008 1.55
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F011 P07-03
F012 1989
F013 A03-03
F016 A01-03: tert-amyl methyl ether (TAME); (CAS #994-05-8)
F020 C15-001
EOB
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B206 PC_WATER_SOL_TAB
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F003 31-07-2006
F004 CLGETTS1
F023 A36-003
F024 1
F007 A02-03
F008 P08-02
F009 5468
F011 25
F020 P09-03:  calculated
F022 A03-02
F025 A01-03: tert-amyl methyl ether (TAME); (CAS #994-05-8)
F030 C14-001
EOB
C
B301 EN_PHOTODEGRADATION_TAB
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F003 04-08-2006
F004 CLGETTS1
F045 A36-003
F046 1
F007 A01-03: tert-amyl methyl ether (TAME); (CAS #994-05-8)
F008 F01-01
F009 F02-05:  Calculated values using AOPWIN version 1.89, a subroutine of the
*    computer program EPI SuiteTM version 3.12
F023 25
F034 F06-03
F035 1500000
F036 F07-02
F044 A02-03
F037 .0000000000052179
F038 A02-03
F040 50
F041 24.6
F042 F05-02
EOR
F001 482
F002 2
F003 01-08-2006
F004 CLGETTS1
F045 A36-003
F046 2
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F007 A01-03: tert-amyl methyl ether (TAME); (CAS #994-05-8)
EOB
C
B302 EN_STABILITY_IN_WATER_TAB
F001 482
F002 1
F003 04-08-2006
F004 CLGETTS1
F040 A36-003
F041 1
F007 A01-03: tert-amyl methyl ether (TAME); (CAS #994-05-8)
F008 F08-01
F009 F09-03:  Technical discussion
F039 A03-02
EOB
C
B305 EN_TRANSPORT_TAB
F001 482
F002 1
F003 31-07-2006
F004 CLGETTS1
F011 A36-003
F012 1
F008 F22-01:  air - biota - sediment(s) - soil - water
F009 F21-01:  Calculation according Mackay, Level I
EOR
F001 482
F002 2
F003 31-07-2006
F004 CLGETTS1
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
C
B308 EN_BIODEGRADATION_TAB
F001 482
F002 1
F003 01-08-2006
F004 CLGETTS1
F047 A36-002
F048 1
F007 A01-03:  tert-amyl methyl ether; CAS #994-05-8
F008 F25-01
F009 F26-18
F011 F27-0141
F017 4
F018 28
F019 F05-01
F020 F30-02:  not readily biodegradable
F046 A03-03
F052 28
F053 F05-01
EOB
```

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C
B310 EN_BIOACCUMULATION_TAB
F001 482
F002 1
F003 04-08-2006
F004 CLGETTS1
F021 A36-003
F022 1
F007 A01-03: tert-amyl methyl ether (TAME); (CAS #994-05-8)
F008 E02-0161:  see remark
F009 F34-06:  calculation
F015 25
F016 A02-03
F017 6
F020 A03-01
EOB
C
B401 EC_FISHTOX_TAB
F001 482
F002 1
F003 01-08-2006
F004 CLGETTS1
F033 A36-002
F034 1
F007 A01-03:  tert-amyl methyl ether (TAME); CAS #994-05-8
F008 E01-02
F009 E02-0101
F010 E03-05:  U.S. Environmental Protection Agency, Methods for acute toxicity
*    testing with fish, macro-invertebrates and amphibians, TSCA § 797.1400
*    (EPA-660/3-75-009)
F011 1987
F012 96
F013 E04-02
F014 E05-02
F021 A02-03
F022 580
F031 A03-03
F032 A03-03
EOR
F001 482
F002 2
F003 31-07-2006
F004 CLGETTS1
F033 A36-003
F034 2
F007 A01-03:  tert-amyl methyl ether; CAS #994-05-8
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 200.6
EOB
C
B402 EC_DAPHNIATOX_TAB
F001 482
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F002 1
F003 01-08-2006
F004 CLGETTS1
F032 A36-002
F033 1
F007 A01-03:  tert-amyl methyl ether (TAME); CAS #994-05-8
F008 E06-0010
F009 E07-04: U.S. Environmental Protection Agency, Methods for acute toxicity
*    testing with fish, macro-invertebrates and amphibians, TSCA § 797.1300
*    (EPA-660/3-75-009).
F010 1975
F011 48
F012 E04-02
F013 E05-02
F020 A02-03
F021 100
F030 A03-03
F031 A03-03
EOR
F001 482
F002 2
F003 31-07-2006
F004 CLGETTS1
F032 A36-003
F033 2
F007 A01-03:  tert-amyl methyl ether; CAS #994-05-8
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 208.4
EOB
C
B403 EC_ALGAETOX_TAB
F001 482
F002 1
F003 01-08-2006
F004 CLGETTS1
F036 A36-002
F037 1
F007 A01-03:  tert-amyl methyl ether (TAME); CAS #994-05-8
F008 E08-0056
F009 E09-03
F011 E10-01
F012 72
F013 E04-02
F014 E05-02
F015 A02-03
F016 77
F030 EbC50
F031 A02-03
F032 230
F034 A03-03
F035 A03-03
F038 ErC50
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F039 A02-03
F040 780
EOR
F001 482
F002 2
F003 31-07-2006
F004 CLGETTS1
F036 A36-003
F037 2
F007 A01-03: tert-amyl methyl ether (TAME); CAS #994-05-8
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 126.9
F030 ChV
F031 A02-03
F032 9.8
EOB
C
B501 TO_ACUTE_ORAL_TAB
F001 482
F002 1
F003 09-10-2006
F004 CLGETTS1
F017 A36-003
F018 1
F007 A01-03: Tertiary Amyl Methyl Ether (TAME) (CAS # 994-05-8)
F008 T01-03
F009 T02-24
F010 T03-03: not specified
F011 1995
F012 A02-06
F013 2100
F015 T04-01
F016 A03-03
F019 T24-03
F021 T52-003: None; administered undiluted
F022 T23-42
EOB
C
B502 TO_ACUTE_INHAL_TAB
F001 482
F002 1
F003 09-10-2006
F004 CLGETTS1
F019 A36-002
F020 1
F007 A01-03: Tertiary Amyl Methyl Ether (TAME) (CAS # 994-05-8)
F008 T05-03
F009 T02-24
F010 T06-03: Not stated
F011 1991
F012 A02-04
F013 5.4

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F015 T07-01
F016 4
F017 T08-01
F018 A03-03
F021 T24-03
F022 10
F023 T52-003:  none
F024 T23-42
F025 5.4 mg/L
EOB
C
B503 TO_ACUTE_DERMAL_TAB
F001 482
F002 1
F003 09-10-2006
F004 CLGETTS1
F017 A36-002
F018 1
F007 A01-03:  Tertiary Amyl Methyl Ether (TAME) (CAS # 994-05-8)
F008 T01-03
F009 T02-23
F010 T09-02:  Limit test; protocol not stated
F011 1985
F012 A02-04
F013 3160
F015 T04-01
F019 T24-03
F020 6
F021 T52-003:  none
F022 T23-31
F023 3160 mg/kg
EOB
C
B507 TO_SENSITIZATION_TAB
F001 482
F002 1
F003 01-08-2006
F004 CLGETTS1
F015 A36-002
F016 1
F007 A01-03:  Tertiary Amyl Methyl Ether (TAME) (CAS:  994-05-8)
F008 T18-14:  Skin sensitization
F009 T02-19:  guinea pig - Dunkin Hartley
F010 T20-03:  TSCA TG 798.4100 (Buehler method)
F011 1995
F012 T47-01
F013 T21-02
F014 A03-03
F030 T52-003:  none
EOB
C
B508 TO_REPEATED_DOSE_TAB
F001 482
F002 1
F003 09-10-2006
F004 CLGETTS1
F030 A36-002
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F031 3
F007 A01-03: Tertiary Amyl Methyl Ether (TAME) (CAS # 994-05-8)
F008 T02-24
F009 T23-16
F010 T24-03
F011 T25-11: Inhalation, whole body
F012 T26-16: TSCA TG 798.2450; US EPA TG 40 CFR Part 798 Subpart G
F013 1997
F014 6 hours/day
F015 5 days/week for 13 weeks (minimum 65 exposures)
F016 4 week recovery period
F017 0, 250, 1500 and 3500 ppm
F018 T27-07
F019 A02-03
F020 1500
F022 T28-05
F032 C07-002
EOR
F001 482
F002 2
F003 09-10-2006
F004 CLGETTS1
F030 A36-002
F031 4
F007 A01-03: Tertiary Amyl Methyl Ether (TAME) (CAS # 994-05-8)
F008 T02-18
F009 T23-10
F010 T24-03
F011 T25-08
F012 T26-16: TSCA TG 798.2450; US EPA TG 40 CFR Part 798 Subpart G
F013 1997
F014 6 hours/day
F015 5 days/week for 13 weeks
F016 4 week recovery period
F017 0, 250, 1500 and 3500 ppm; due to high incidence of mortality at 3500 ppm
*   early in the study, the high dose was eventually set at 2500 ppm (i.e.,
*   new high dose and control groups were established)
F018 T27-07
F019 A02-03
F020 1500
F022 T28-05
F029 A03-03
F032 C07-002
EOR
F001 482
F002 3
F003 09-10-2006
F004 CLGETTS1
F030 A36-003
F031 1
F007 A01-03: Tertiary Amyl Methyl Ether (TAME) (CAS # 994-05-8)
F008 T02-24
F009 T23-42
F010 T24-03
F011 T25-11: Inhalation, whole body
F013 1995
F014 6 hours/day

F015 5 days/week for 4 weeks
F016 18 hour fasting period
F017 0, 500, 2000 and 4000 ppm
F018 T27-07
F019 A02-03
F020 500
F022 T28-05
F032 C07-002
EOR
F001 482
F002 4
F003 09-10-2006
F004 CLGETTS1
F030 A36-002
F031 2
F007 A01-03: Tertiary Amyl Methyl Ether (TAME) (CAS # 994-05-8)
F008 T02-24
F009 T23-42
F010 T24-03
F011 T25-11: Oral, gavage
F012 T26-16
F013 1995
F015 7 days/week for 29 days
F017 0, 125, 500 and 1000 mg/kg/day
F018 T27-07
F019 A02-03
F020 500
F022 T28-02
F029 A03-03
F032 C07-002
EOB
C
B509 TO_GENETIC_IN_VITRO_TAB
F001 482
F002 1
F003 09-10-2006
F004 CLGETTS1
F016 A36-002
F017 1
F007 A01-03: Tertiary Amyl Methyl Ether (TAME) (CAS # 994-05-8)
F008 T30-05
F009 T31-18: EPA OTS 798.5265, Similar to OECD Guideline 471
F010 1995
F011 Salmonella typhimurium
F012 T32-03
F013 T33-02
F014 A03-03
F015 Doses ranging from 100 to 10,000 ug per plate
F018 >10,000 ug/plate
EOR
F001 482
F002 2
F003 09-10-2006
F004 CLGETTS1
F016 A36-002
F017 2
F007 A01-03: Tertiary Amyl Methyl Ether (TAME) (CAS # 994-05-8)

F008 T30-19: Mammalian Chromosomal Aberration Test
F009 T31-18: OECD Guideline 473
F010 1997
F011 Chinese hamster ovary cells (CHO)
F012 T32-03
F013 T33-03
F014 A03-02
F015 313, 625, 1250, 2500 and 5000 ug/ml
F018 5000 ug/ml
EOB
C
B510 TO_GENETIC_IN_VIVO_TAB
F001 482
F002 1
F003 09-10-2006
F004 CLGETTS1
F018 A36-002
F019 1
F007 A01-03: Tertiary Amyl Methyl Ether (TAME) (CAS # 994-05-8)
F008 T34-12: Mammalian Erythrocyte Micronucleus Test
F009 T02-18
F010 T23-10
F011 T37-15: EPA OTS 798.5395, Similar to OECD Guideline 474
F012 1995
F013 T24-03
F014 T25-11: Intraperitoneal injection
F015 Bone marrow (femur) sampled at 24hr, 48hr, 72hr after administration
*   (24hr only for the positive control substance)
F016 0.15, 0.375, 0.75 g/kg
F017 A03-03
F020 T33-02
EOB
C
B512 TO_REPRODUCTION_TAB
F001 482
F002 1
F003 09-10-2006
F004 CLGETTS1
F037 A36-002
F038 1
F007 A01-03: Tertiary Amyl Methyl Ether (CAS # 994-05-8)
F008 T41-04: Two-generation Reproductive Toxicity Test
F009 T02-24
F010 T23-42
F011 T24-03
F012 T25-11: Whole body inhalation
F036 Males: premating, mating, postmating (30 days); Females: premating,
*   mating through gestational day 19, lactation (postnatal day 5 through 28)
F013 T40-05: OPPTS - 1996 draft guidelines
F014 2003
F015 6 hr/day, 5-7 days/week
F016 5 days/week for 10 weeks
F017 5 days/week for 10 weeks
F018 43 weeks
F019 250, 1500 and 3000 ppm
F020 T27-03: Yes - air-exposed
F035 A03-03

F054 2
EOB
C
B513 TO_DEVELOPMENTAL_TAB
F001 482
F002 1
F003 09-10-2006
F004 CLGETTS1
F030 A36-002
F031 1
F007 A01-03: Tertiary Amyl Methyl Ether (TAME) (CAS # 994-05-8)
F008 T02-24
F009 T23-42
F010 T24-01
F011 T25-08
F012 T44-03: EPA OPPTS - 1996 draft guidelines
F013 2003
F014 14 days
F015 6 hr/day
F016 Gestation Days 6-19 (14 consecutive days)
F017 0, 250, 1500, or 3500 ppm
F018 T27-03: yes (air-exposed)
F019 A02-03
F020 250
F022 T43-04
F029 A03-03
F032 T58-007: NOAEL Pupl
F033 A02-03
F034 1500
F036 T43-04
F047 Maternal NOAEL: 250 ppm; Pup NOAEL: 1500 ppm
EOR
F001 482
F002 2
F003 09-10-2006
F004 CLGETTS1
F030 A36-002
F031 2
F007 A01-03: Tertiary Amyl Methyl Ether (TAME) (CAS # 994-05-8)
F008 T02-18
F009 T23-10
F010 T24-01
F011 T25-08
F012 T44-03: EPA OPPTS - 1996 draft guidelines
F013 2003
F014 11 days
F015 6 hr/day
F016 Gestation Days 6-16 (11 consecutive days)
F017 0, 250, 1500, or 3500 ppm
F018 T27-03: yes (air-exposed)
F019 A02-03
F020 250
F022 T43-04
F029 A03-03
F032 T58-007: NOAEL Pup
F033 A02-03
F034 250

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F036 T43-04
F047 Maternal NOAEL: 250 ppm;  Pup NOAEL: 250 ppm
EOB
C
B601 TEXT_TAB
F002 482
F010 2.1
F004 1
F005 ME
F006 Melting Point is calculated by the MPBPWIN, version 1.41, a subroutine of
*    the computer program EPI SuiteTM, version 3.012, (2000) which is based on
*    the average result of the methods of K. Joback and Gold and Ogle.
**
**   Joback's Method is descri
F007 Melting Point is calculated by the MPBPWIN, version 1.41, a subroutine of
*    the computer program EPI SuiteTM, version 3.012, (2000) which is based on
*    the average result of the methods of K. Joback and Gold and Ogle.
**
**   Joback's Method is described in Joback K (1982). A Unified Approach to
*    Physical Property Estimation Using Multivariate Statistical Techniques.
*    In The Properties of Gases and Liquids. Fourth Edition. (1987). R Reid, J
*    Prausnitz and B 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 258639
EOR
F002 482
F010 2.1
F004 1
F005 RE
F006 U.S. Environmental Protection Agency (U.S. EPA) (2000). EPI SuiteTM,
*    Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.
F007 U.S. Environmental Protection Agency (U.S. EPA) (2000). EPI SuiteTM,
*    Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.
F020 258642
EOR
F002 482
F010 2.1
F004 1
F005 RL
F006 The value was calculated based on chemical structure as modeled by EPI
*    SuiteTM.  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 EPI
*    SuiteTM.  This robust summary has a reliability rating of 2 because the
*    data are calculated and not measured.
F020 258641
EOR
F002 482
F010 2.1
F004 1
F005 TS
F006 CAS #994-05-8; tert-amyl methyl ether
F007 CAS #994-05-8; tert-amyl methyl ether
F020 258640
```

EOR
F002 482
F010 2.2
F004 1
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 258645
EOR
F002 482
F010 2.2
F004 1
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 258644
EOR
F002 482
F010 2.2
F004 1
F005 TS
F006 CAS #994-05-8; tert-amyl methyl ether; purity is unknown.
F007 CAS #994-05-8; tert-amyl methyl ether; purity is unknown.
F020 258643
EOR
F002 482
F010 2.3
F004 1
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 258648
EOR
F002 482
F010 2.3
F004 1
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 258647
EOR
F002 482
F010 2.3
F004 1
F005 TS

F006 CAS #994-05-8; tert-amyl methyl ether; purity is unknown.
F007 CAS #994-05-8; tert-amyl methyl ether; purity is unknown.
F020 258646
EOR
F002 482
F010 2.4
F004 1
F005 ME
F006 Neste Company method 205 using Grabner apparatus.
F007 Neste Company method 205 using Grabner apparatus.
F020 258649
EOR
F002 482
F010 2.4
F004 1
F005 RE
F006 Huttunen H (1996). Risk assessment of complex petroleum substances:
* hazard identification of NExTAME and re-formulated gasoline. Licentiate's
* Thesis, University of Kuopio, April 1996.
F007 Huttunen H (1996). Risk assessment of complex petroleum substances:
* hazard identification of NExTAME and re-formulated gasoline. Licentiate's
* Thesis, University of Kuopio, April 1996.
F020 258653
EOR
F002 482
F010 2.4
F004 1
F005 RE
F006 Huttunen H, Wyness L and Kalliokoski P (1997). Identification of the
* environmental hazards of gasoline oxygenate tert-amyl methyl ether
* (TAME). Chemosphere 35, 1199-1214.
F007 Huttunen H, Wyness L and Kalliokoski P (1997). Identification of the
* environmental hazards of gasoline oxygenate tert-amyl methyl ether
* (TAME). Chemosphere 35, 1199-1214.
F020 258654
EOR
F002 482
F010 2.4
F004 1
F005 RL
F006 This robust summary has a reliability rating of 2 because the data were
* not reviewed for quality. These data were used for the vapor pressure
* endpoint in the European Union Risk Assessment for tert-amyl methyl ether
* (Finnish Environment Ins
F007 This robust summary has a reliability rating of 2 because the data were
* not reviewed for quality. These data were used for the vapor pressure
* endpoint in the European Union Risk Assessment for tert-amyl methyl ether
* (Finnish Environment Institute (2004). 2-Methoxy-Methyl Butane (TAME)
* Environmental Risk Assessment. Final Draft.).
F020 258652
EOR
F002 482
F010 2.4
F004 1
F005 RM
F006 Mean of duplicate determinations, SD = 6
F007 Mean of duplicate determinations, SD = 6

F020 258651
EOR
F002 482
F010 2.4
F004 1
F005 TS
F006 CAS #994-05-8; tert-amyl methyl ether; purity is unknown.
F007 CAS #994-05-8; tert-amyl methyl ether; purity is unknown.
F020 258650
EOR
F002 482
F010 2.4
F004 2
F005 ME
F006 Estimated value, interpolated from measured data (various sources)
F007 Estimated value, interpolated from measured data (various sources)
F020 258655
EOR
F002 482
F010 2.4
F004 2
F005 RE
F006 Huttunen H (1996). Risk assessment of complex petroleum substances:
*   hazard identification of NExTAME and re-formulated gasoline. Licentiate's
*   Thesis, University of Kuopio, April 1996.
F007 Huttunen H (1996). Risk assessment of complex petroleum substances:
*   hazard identification of NExTAME and re-formulated gasoline. Licentiate's
*   Thesis, University of Kuopio, April 1996.
F020 258658
EOR
F002 482
F010 2.4
F004 2
F005 RE
F006 Huttunen H, Wyness L and Kalliokoski P (1997). Identification of the
*   environmental hazards of gasoline oxygenate tert-amyl methyl ether
*   (TAME). Chemosphere 35, 1199-1214.
F007 Huttunen H, Wyness L and Kalliokoski P (1997). Identification of the
*   environmental hazards of gasoline oxygenate tert-amyl methyl ether
*   (TAME). Chemosphere 35, 1199-1214.
F020 258659
EOR
F002 482
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. These data were used for the vapor pressure
*   endpoint in the European Union Risk Assessment for tert-amyl methyl ether
*   (Finnish Environment Ins
F007 This robust summary has a reliability rating of 2 because the data were
*   not reviewed for quality. These data were used for the vapor pressure
*   endpoint in the European Union Risk Assessment for tert-amyl methyl ether
*   (Finnish Environment Institute (2004). 2-Methoxy-Methyl Butane (TAME)
*   Environmental Risk Assessment. Final Draft.).
F020 258657
EOR

F002 482
F010 2.4
F004 2
F005 TS
F006 CAS #994-05-8; tert-amyl methyl ether
F007 CAS #994-05-8; tert-amyl methyl ether
F020 258656
EOR
F002 482
F010 2.4
F004 3
F005 ME
F006 Neste Method 103 using SETVAC apparatus.
F007 Neste Method 103 using SETVAC apparatus.
F020 258660
EOR
F002 482
F010 2.4
F004 3
F005 RE
F006 Huttunen H (1996). Risk assessment of complex petroleum substances:
* hazard identification of NExTAME and re-formulated gasoline. Licentiate's
* Thesis, University of Kuopio, April 1996.
F007 Huttunen H (1996). Risk assessment of complex petroleum substances:
* hazard identification of NExTAME and re-formulated gasoline. Licentiate's
* Thesis, University of Kuopio, April 1996.
F020 258664
EOR
F002 482
F010 2.4
F004 3
F005 RL
F006 This robust summary has a reliability rating of 2 because the data were
* not reviewed for quality. These data were used for the vapor pressure
* endpoint in the European Union Risk Assessment for tert-amyl methyl
* ether(Finnish Environment Inst
F007 This robust summary has a reliability rating of 2 because the data were
* not reviewed for quality. These data were used for the vapor pressure
* endpoint in the European Union Risk Assessment for tert-amyl methyl
* ether(Finnish Environment Institute (2004). 2-Methoxy-Methyl Butane
* (TAME) Environmental Risk Assessment. Final Draft.).
F020 258663
EOR
F002 482
F010 2.4
F004 3
F005 RM
F006 Mean of duplicate determinations, SD = 10
F007 Mean of duplicate determinations, SD = 10
F020 258662
EOR
F002 482
F010 2.4
F004 3
F005 TS
F006 CAS #994-05-8; tert-amyl methyl ether; purity is unknown.
F007 CAS #994-05-8; tert-amyl methyl ether; purity is unknown.

F020 258661
EOR
F002 482
F010 2.5
F004 1
F005 ME
F006 Mean of six determinations. SD = 0.021 water : octanol ratios of 1:2, 1:1
* and 2:1 were used, and the concentration of TAME determined by gas
* chromatography after through mixing of the two phases. Volatilisation was
* controlled by sealed vial
F007 Mean of six determinations. SD = 0.021 water : octanol ratios of 1:2, 1:1
* and 2:1 were used, and the concentration of TAME determined by gas
* chromatography after through mixing of the two phases. Volatilisation was
* controlled by sealed vials and gas tight syringes.
F020 258665
EOR
F002 482
F010 2.5
F004 1
F005 RE
F006 Huttunen H (1996). Risk assessment of complex petroleum substances:
* hazard identification of NExTAME and re-formulated gasoline. Licentiate's
* Thesis, University of Kuopio, April 1996.
F007 Huttunen H (1996). Risk assessment of complex petroleum substances:
* hazard identification of NExTAME and re-formulated gasoline. Licentiate's
* Thesis, University of Kuopio, April 1996.
F020 258668
EOR
F002 482
F010 2.5
F004 1
F005 RE
F006 Huttunen H, Wyness L and Kalliokoski P (1997). Identification of the
* environmental hazards of gasoline oxygenate tert-amyl methyl ether
* (TAME). Chemosphere 35, 1199-1214.
F007 Huttunen H, Wyness L and Kalliokoski P (1997). Identification of the
* environmental hazards of gasoline oxygenate tert-amyl methyl ether
* (TAME). Chemosphere 35, 1199-1214.
F020 258669
EOR
F002 482
F010 2.5
F004 1
F005 RE
F006 Russell S (1995). TAME: Determination of physico chemical properties.
* Hazleton Report 1359/1-1014. September 1995 (Neste Oil Refining Report RR
* 58/95).
F007 Russell S (1995). TAME: Determination of physico chemical properties.
* Hazleton Report 1359/1-1014. September 1995 (Neste Oil Refining Report RR
* 58/95).
F020 258670
EOR
F002 482
F010 2.5
F004 1
F005 RL
F006 The value cited by the authors is a measured and preferred value. This

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*    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 258667
EOR
F002 482
F010 2.5
F004 1
F005 TS
F006 CAS #994-05-8; tert-amyl methyl ether; purity is unknown.
F007 CAS #994-05-8; tert-amyl methyl ether; purity is unknown.
F020 258666
EOR
F002 482
F010 2.6.1
F004 1
F005 RE
F006 U.S. Environmental Protection Agency (U.S. EPA) (2000). EPI SuiteTM,
*    Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.
F007 U.S. Environmental Protection Agency (U.S. EPA) (2000). EPI SuiteTM,
*    Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.
F020 258674
EOR
F002 482
F010 2.6.1
F004 1
F005 RL
F006 The value was calculated based on chemical structure as modeled by EPI
*    SuiteTM (2000).  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 EPI
*    SuiteTM (2000).  This robust summary has a reliability rating of 2
*    because the data are calculated and not measured.
F020 258673
EOR
F002 482
F010 2.6.1
F004 1
F005 TC
F006 Water Solubility is calculated by the WSKOW, version 1.41, a subroutine
*    of the computer program EPI SuiteTM, version 3.12, which is based on a
*    Kow correlation method described by W. Meylan, P. Howard and R. Boethling
*    in "Improved method for
F007 Water Solubility is calculated by the WSKOW, version 1.41, a subroutine
*    of the computer program EPI SuiteTM, version 3.12, which is 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.
**   A log Kow of 1.55 was used with the model.
F020 258671
EOR
F002 482
F010 2.6.1
F004 1
F005 TS
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F006 CAS #994-05-8; tert-amyl methyl ether
F007 CAS #994-05-8; tert-amyl methyl ether
F020 258672
EOR
F002 482
F010 3.1.1
F004 1
F005 ME
F006 Calculated values using AOPWIN version 1.89, a subroutine of the computer
*   program EPI SuiteTM version 3.12
**
**   Indirect photodegradation, or atmospheric oxidation potential, is based
*   on the structure-activity relationship methods developed by
F007 Calculated values using AOPWIN version 1.89, a subroutine of the computer
*   program EPI SuiteTM 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 258675
EOR
F002 482
F010 3.1.1
F004 1
F005 RE
F006 U.S. Environmental Protection Agency (U.S. EPA) (2000). EPI SuiteTM,
*   Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.
F007 U.S. Environmental Protection Agency (U.S. EPA) (2000). EPI SuiteTM,
*   Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.
F020 258679
EOR
F002 482
F010 3.1.1
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 258677
EOR
F002 482
F010 3.1.1
F004 1
F005 RM
F006 Tertiary-amyl methyl ether has the potential to volatilize to air, based
*   on a relatively high vapor pressure, where it is subject to atmospheric
*   oxidation. In air, tert-amyl methyl ether can react with photosensitized
*   oxygen in the form of
F007 Tertiary-amyl methyl ether has the potential to volatilize to air, based
*   on a relatively high vapor pressure, where it is subject to atmospheric
*   oxidation. In air, tert-amyl methyl ether can react with photosensitized

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*    oxygen in the form of hydroxyl radicals (OH-). The computer program
*    AOPWIN (atmospheric oxidation program for Microsoft Windows) (EPI
*    SuiteTM, 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.
**   Based on a 12-hour day, a rate constant of 5.22 E-12 cm3/molecule*sec,
*    and an OH- concentration of 1.5 E6 OH-/cm3, tertiary-amyl methyl ether
*    has a calculated half-life in air of 2.05 days or 24.6 hours of daylight.
F020 258676
EOR
F002 482
F010 3.1.1
F004 1
F005 TS
F006 CAS #994-05-8; tert-amyl methyl ether
F007 CAS #994-05-8; tert-amyl methyl ether
F020 258678
EOR
F002 482
F010 3.1.1
F004 2
F005 ME
F006 Technical discussion
F007 Technical discussion
F020 258680
EOR
F002 482
F010 3.1.1
F004 2
F005 RE
F006 Harris J (1982). Rate of Aqueous Photolysis. In: Handbook of Chemical
*    Property Estimation Methods. Chapter 8. Edited by WJ Lyman, WF Reehl and
*    DH Rosenblatt. McGraw-Hill Book Company, New York, NY, USA.
F007 Harris J (1982). Rate of Aqueous Photolysis. In: Handbook of Chemical
*    Property Estimation Methods. Chapter 8. Edited by WJ Lyman, WF Reehl and
*    DH Rosenblatt. McGraw-Hill Book Company, New York, NY, USA.
F020 258684
EOR
F002 482
F010 3.1.1
F004 2
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 258685
EOR
F002 482
F010 3.1.1
F004 2
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
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*    discussion and not a study.
F020 258682
EOR
F002 482
F010 3.1.1
F004 2
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, 1982).
**   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, tert-amyl methyl ether is not subject to photolytic
*    processes in the aqueous environment.
F020 258681
EOR
F002 482
F010 3.1.1
F004 2
F005 TS
F006 CAS #994-05-8; tert-amyl methyl ether
F007 CAS #994-05-8; tert-amyl methyl ether
F020 258683
EOR
F002 482
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 258689
EOR
F002 482
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
```

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*    Rosenblatt. McGraw-Hill Book Company, New York, NY, USA.
F020 258690
EOR
F002 482
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 258687
EOR
F002 482
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. Tertiary amyl methyl ether is resistant to hydrolysis
*    because it lacks a functional group that is hydrolytically reactive and
*    Harris (1982) identifies ether groups as generally resistant to
*    hydrolysis. Therefore, hydrolysis will not contribute to the removal of
*    tert-amyl methyl ether from the environment.
F020 258686
EOR
F002 482
F010 3.1.2
F004 1
F005 TS
F006 CAS #994-05-8; tert-amyl methyl ether
F007 CAS #994-05-8; tert-amyl methyl ether
F020 258688
EOR
F002 482
F010 3.3.1
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.
F020 258695
EOR
F002 482
F010 3.3.1
F004 1
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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 258694
EOR
F002 482
F010 3.3.1
F004 1
F005 RM
F006 Physicochemical data used in the calculation:
**
**   Parameter   Value w/ Units
**
**   Molecular Weight = 102.18
**   Temperature =   25° C
**   Log Kow =   1.55
**   Water Solubility = 5468 g/m3
**   Vapor Pressure =   12,000 Pa
**   Melting Point =   -81.22° C
F007 Physicochemical data used in the calculation:
**
**   Parameter   Value w/ Units
**
**   Molecular Weight = 102.18
**   Temperature =   25° C
**   Log Kow =   1.55
**   Water Solubility = 5468 g/m3
**   Vapor Pressure =   12,000 Pa
**   Melting Point =   -81.22° C
F020 258692
EOR
F002 482
F010 3.3.1
F004 1
F005 RS
F006 Using the Mackay Level I calculation, the following
**   distribution is predicted for tert-amyl methyl ether:
**
**   %Distribution Compartment
**   97.77   Air
**   2.16   Water
**   0.07   Soil
**   <0.01   Sediment
**   <0.01   Suspended Sediment
**   <0.01   Biota
F007 Using the Mackay Level I calculation, the following
**   distribution is predicted for tert-amyl methyl ether:
**
**   %Distribution Compartment
**   97.77   Air
**   2.16   Water
**   0.07   Soil
**   <0.01   Sediment
**   <0.01   Suspended Sediment
**   <0.01   Biota

F020 258693
EOR
F002 482
F010 3.3.1
F004 1
F005 TS
F006 CAS #994-05-8; tert-amyl methyl ether
F007 CAS #994-05-8; tert-amyl methyl ether
F020 258691
EOR
F002 482
F010 3.3.1
F004 2
F005 CL
F006 The majority of tert-amyl methyl ether (TAME) 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. TAME is
*   considered to be a Typ
F007 The majority of tert-amyl methyl ether (TAME) 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. TAME is
*   considered to be a Type 1 chemical with potential to partition into all
*   environmental compartments.
F020 258700
EOR
F002 482
F010 3.3.1
F004 2
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 cannot
*   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.

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*    The advective residence time of aerosols, suspended sediment and fish
*    cannot be specified independently of the air and water residence times.
F020 258696
EOR
F002 482
F010 3.3.1
F004 2
F005 RE
F006 Mackay D (1998). Level III Fugacity-Based Environmental Equilibrium
*    Partitioning Model, Version 2.1 (16-bit). Environmental Modelling Centre,
*    Trent University, Ontario, Canada.
F007 Mackay D (1998). Level III Fugacity-Based Environmental Equilibrium
*    Partitioning Model, Version 2.1 (16-bit). Environmental Modelling Centre,
*    Trent University, Ontario, Canada.
F020 258702
EOR
F002 482
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 258701
EOR
F002 482
F010 3.3.1
F004 2
F005 RS
F006 Output:
**          Mass% Emissions(kg/hr)
**   Air          26.2  1000
**   Water        55.1  1000
**   Soil         18.6  1000
**   Sediment     0.1   0
F007 Output:
**          Mass% Emissions(kg/hr)
**   Air          26.2  1000
**   Water        55.1  1000
**   Soil         18.6  1000
**   Sediment     0.1   0
F020 258697
EOR
F002 482
F010 3.3.1
F004 2
F005 TC
F006 Physicochemical data used in the calculation:
**
**   Parameter         Value w/ Units
**
**   Molecular Weight = 102.18
**   Temperature =            25° C
**   Log Kow =          1.55
**   Water Solubility = 5468 g/m3
**   Vapor Pressure =   12,000 Pa
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**   Melting Point =          -81.22° C
**
**   Reaction Hal
F007 Physicochemical data used in the calculation:
**
**   Parameter         Value w/ Units
**
**   Molecular Weight = 102.18
**   Temperature =            25° C
**   Log Kow =          1.55
**   Water Solubility = 5468 g/m3
**   Vapor Pressure =   12,000 Pa
**   Melting Point =          -81.22° C
**
**   Reaction Half Lives in hours as predicted using EPI SuiteTM:
**
**   Air (gaseous)            46.7
**   Water (no susp. part.)   360
**   Bulk Soil          720
**   Bulk Sediment            3240
**
**   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 258698
EOR
F002 482
F010 3.3.1
F004 2
F005 TS
F006 CAS #994-05-8; tert-amyl methyl ether
F007 CAS #994-05-8; tert-amyl methyl ether
F020 258699
EOR
F002 482
F010 3.5
F004 1
F005 CL
F006 tert-Amyl methyl ether is not readily biodegradable.
F007 tert-Amyl methyl ether is not readily biodegradable.
F020 258705
EOR
F002 482
F010 3.5
F004 1
F005 RE
F006 Bealing D (1995). Tertiary amyl methyl ether (TAME): assessment of ready
*    biodegradability by measurement of oxygen uptake. Hazleton Europe. Report
*    No. 1359/3-1018. 28 February 1995.
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F007 Bealing D (1995). Tertiary amyl methyl ether (TAME): assessment of ready
*    biodegradability by measurement of oxygen uptake. Hazleton Europe. Report
*    No. 1359/3-1018. 28 February 1995.
F020 258707
EOR
F002 482
F010 3.5
F004 1
F005 RS
F006 4.0% degradation was observed after 28 days incubation with an
*    unacclimated inoculum. >60% Degradation of the control substance (sodium
*    benzoate) occurred within 10 days, indicating that the test was valid.
**   % Biodegradation of test substanc
F007 4.0% degradation was observed after 28 days incubation with an
*    unacclimated inoculum. >60% Degradation of the control substance (sodium
*    benzoate) occurred within 10 days, indicating that the test was valid.
**   % Biodegradation of test substance after days:
**   2 days = 0 %
**   7 days = 5 %
**   14 days      = 4 %
**   21 days      = 4 %
**   28 days      = 4 %
**
**   % Biodegradation of positive control, Benzoic acid, sodium salt:
**   2 days = 52 %
**   7 days = 77 %
F020 258703
EOR
F002 482
F010 3.5
F004 1
F005 TC
F006 OECD Guideline 301 D "Ready Biodegradability: Closed Bottle Test",  using
*    1.99 ± 0.03 mg/l of test substance.
F007 OECD Guideline 301 D "Ready Biodegradability: Closed Bottle Test",  using
*    1.99 ± 0.03 mg/l of test substance.
F020 258704
EOR
F002 482
F010 3.5
F004 1
F005 TS
F006 CAS #994-05-8; tert-amyl methyl ether; purity unknown.
F007 CAS #994-05-8; tert-amyl methyl ether; purity unknown.
F020 258706
EOR
F002 482
F010 3.7
F004 1
F005 RE
F006 ECOSAR v0.99h (2004) in EPI SuiteTM, U.S. EPA (2000). Estimation Program
*    Interface Suite, v3.12. Syracuse Research Corporation, Syracuse, NY, USA.
F007 ECOSAR v0.99h (2004) in EPI SuiteTM, U.S. EPA (2000). Estimation Program
*    Interface Suite, v3.12. Syracuse Research Corporation, Syracuse, NY, USA.
F020 258711
EOR
F002 482
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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 258709
EOR
F002 482
F010 3.7
F004 1
F005 RM
F006 A log bioconcentration factor (BCF) of 0.78 is calculated (BCF = 6.0).
* With respect to a log Kow = 1.92, which was used to calculate the BCF,
* tert-amyl methyl ether in the aquatic environment is expected to have a
* low bioaccumulation potent
F007 A log bioconcentration factor (BCF) of 0.78 is calculated (BCF = 6.0).
* With respect to a log Kow = 1.92, which was used to calculate the BCF,
* tert-amyl methyl ether in the aquatic environment is expected to have a
* low bioaccumulation potential.
F020 258708
EOR
F002 482
F010 3.7
F004 1
F005 TS
F006 CAS #994-05-8; tert-amyl methyl ether
F007 CAS #994-05-8; tert-amyl methyl ether
F020 258710
EOR
F002 482
F010 4.1
F004 1
F005 ME
F006 The test guideline followed was TSCA § 797.1400. Twenty organisms (ten
* per replicate) were exposed in duplicate test aquaria to each of five
* concentrations of TAME and a dilution water control for 96-hours. During
* the test, nominal concentr
F007 The test guideline followed was TSCA § 797.1400. Twenty organisms (ten
* per replicate) were exposed in duplicate test aquaria to each of five
* concentrations of TAME and a dilution water control for 96-hours. During
* the test, nominal concentrations of 950, 570, 340, 210, and 120 mg A.I./L
* were maintained by introducing approximately 6.5 aquarium volumes per day
* of newly prepared test dilution via a modified constant-flow serial
* diluter apparatus. Each replicate solution was sampled and analyzed for
* TAME concentration at 0 hours and after 96 hours of exposure. Based on
* the results of these analyses, the mean measured exposure concentrations
* were defined as 640, 560, 310, 150, and 78 mg A.I./L. Biological
* observations and observations of the physical characteristics of the
* exposure solutions were made and recorded at test initiation and every 24
* hours thereafter until the test was terminated. Throughout the exposure
* period, treatment level solution were observed to be clear and colorless
* and contained no visible sign of undissolved test material. Test vessels
* were not covered during the exposure period.
F020 258712
EOR

F002 482
F010 4.1
F004 1
F005 RE
F006 American Petroleum Institute (1995). Tert-Amyl Methyl Ether (TAME) -
*   Acute Toxicity to Rainbow Trout (Oncorhynchus mykiss) Under Flow-through
*   Conditions. Toxicology Report Number 408. Springborn Laboratories, Inc.
*   SLI Report 93-3-4682.
F007 American Petroleum Institute (1995). Tert-Amyl Methyl Ether (TAME) -
*   Acute Toxicity to Rainbow Trout (Oncorhynchus mykiss) Under Flow-through
*   Conditions. Toxicology Report Number 408. Springborn Laboratories, Inc.
*   SLI Report 93-3-4682.
F020 258717
EOR
F002 482
F010 4.1
F004 1
F005 RL
F006 Guideline study that followed GLP.
F007 Guideline study that followed GLP.
F020 258716
EOR
F002 482
F010 4.1
F004 1
F005 RM
F006 Statistics: The LC50 was estimated by nonlinear interpolation and 95%
*   confidence intervals were calculated by bionomial probability.
F007 Statistics: The LC50 was estimated by nonlinear interpolation and 95%
*   confidence intervals were calculated by bionomial probability.
F020 258713
EOR
F002 482
F010 4.1
F004 1
F005 RS
F006 96-hour LC50 = 580 mg/L based on mean measured values.
**   72-hour LC50 = 580 mg/L based on mean measured values.
**   48-hour LC50 = 600 mg/L based on mean measured values.
**   24-hour LC50 = 600 mg/L based on mean measured values.
**   96-hour NOEC = 310 m
F007 96-hour LC50 = 580 mg/L based on mean measured values.
**   72-hour LC50 = 580 mg/L based on mean measured values.
**   48-hour LC50 = 600 mg/L based on mean measured values.
**   24-hour LC50 = 600 mg/L based on mean measured values.
**   96-hour NOEC = 310 mg/L based on mean measured values.
**
**   After 72-hours of exposure, 100% mortality was observed among fish
*   exposed to the highest mean measured concentration tested (640 mg/L). At
*   test termination (96 hours), 30% mortality was observed among fish
*   exposed to the 560 mg/L treatment level. In addition, sublethal effects,
*   as defined by darkened pigmentation and equilibrium loss, were observed
*   among all of the surviving fish exposed to this treatment level. No
*   mortality or sublethal effects were observed among fish exposed to the
*   remaining concentrations tested. The NOEC established during this study
*   was 310 mg/L, based on darkened pigmentation and equilibrium loss. There
*   was no control mortality through the test period.

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**
**   Analytical results:
**   Nominal treatment levels of 950, 570, 340, 210, and 120 mg A.I./L
*    measured 640, 560, 310, 150, and 78 mg  A.I./L, respectively. Both 0- and
*    96-hour control samples measured <5.3 mg  A.I./L. Mean measured
*    concentrations averaged 79% of the nominal concentrations. Coefficients
*    of variation averaged 12% for all mean measured concentrations.
**
**   Water quality parameter results:
**   Temperature ranged between 11 to 12°C through the 96-hour exposure. The
*    pH was 7.1 in all treatment levels and the control at time 0, and pH was
*    7.2 in all treatment levels and the control at the 24, 48, 72, and
*    96-hour samplings. Dissolved oxygen ranged from 9.6 to 9.8 mg/L in all
*    treatment levels and the control at time 0, 9.4 to 9.6 mg/L in all
*    treatment levels and the control at time 24, 9.0 to 9.4 mg/L in all
*    treatment levels and the control at time 48, 9.4 to 9.8 mg/L in all
*    treatment levels and the control at time 72, and 8.9 to 9.1 mg/L in all
*    treatment levels and the control at time 96.
F020 258714
EOR
F002 482
F010 4.1
F004 1
F005 TS
F006 CAS #994-05-8; tert-amyl methyl ether; 98.8% purity
F007 CAS #994-05-8; tert-amyl methyl ether; 98.8% purity
F020 258715
EOR
F002 482
F010 4.1
F004 2
F005 ME
F006 ECOSAR version 0.99h, U.S. 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 h
F007 ECOSAR version 0.99h, U.S. 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
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*    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 258718
EOR
F002 482
F010 4.1
F004 2
F005 RE
F006 U.S. Environmental Protection Agency (U.S. EPA) (2000). EPI SuiteTM,
*    Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.
F007 U.S. Environmental Protection Agency (U.S. EPA) (2000). EPI SuiteTM,
*    Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.
F020 258723
EOR
F002 482
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 258722
EOR
F002 482
F010 4.1
F004 2
F005 RS
F006 Calculated 96-hr LC50 for fish = 200.6 mg/L
F007 Calculated 96-hr LC50 for fish = 200.6 mg/L
F020 258719
EOR
F002 482
F010 4.1
F004 2
F005 TC
F006 Experimental water solubility, 5468 mg/l @ 20°C (U.S. EPA, 2000), log
*    Kow, 1.55 (Huttunen et al., 1997) and melting point, -82.1°C (U.S. EPA,
*    2000) were entered into the program.
**   Class: Neutral organics
F007 Experimental water solubility, 5468 mg/l @ 20°C (U.S. EPA, 2000), log
*    Kow, 1.55 (Huttunen et al., 1997) and melting point, -82.1°C (U.S. EPA,
*    2000) were entered into the program.
**   Class: Neutral organics
F020 258720
EOR
F002 482
F010 4.1
F004 2
F005 TS
F006 CAS #994-05-8; tert-amyl methyl ether
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F007 CAS #994-05-8; tert-amyl methyl ether
F020 258721
EOR
F002 482
F010 4.2
F004 1
F005 ME
F006 The test guideline followed was TSCA § 797.1300. Twenty organisms (ten
* per replicate) were exposed in duplicate test vessels to five
* concentrations of TAME and a dilution water control for 48 hours. During
* the test, nominal concentrations
F007 The test guideline followed was TSCA § 797.1300. Twenty organisms (ten
* per replicate) were exposed in duplicate test vessels to five
* concentrations of TAME and a dilution water control for 48 hours. During
* the test, nominal concentrations of 690, 410, 250, 150, and 89 mg A.I./L
* were maintained in the exposure vessels by introducing approximately 6.0
* test chamber volumes per day of newly prepared test solution via an
* intermittent-flow proportional diluter apparatus. Each replicate solution
* was sampled and analyzed for TAME concentration at 0 hours (test
* initiation) and after 48 hours (test termination) of the exposure period.
* Based on the results of these analyses, the mean measured exposure
* concentrations were defined as 120, 83, 55, 28, and 15 mg/l. Biological
* observations and observations of the physical characteristics of the
* exposure solutions were made and recorded at test initiation, 6, 24, and
* 48 hours. Throughout the exposure period, no visible signs of undissolved
* test material were observed in either the diluter system or in the
* exposure solutions.
F020 258724
EOR
F002 482
F010 4.2
F004 1
F005 RE
F006 American Petroleum Institute (1994). Tert-Amyl Methyl Ether (TAME) -
* Acute Toxicity to Daphnids (Daphnia magna) Under Flow-through Conditions.
* Toxicology Report Number 408. Springborn Laboratories, Inc. SLI Report
* 92-12-4545.
F007 American Petroleum Institute (1994). Tert-Amyl Methyl Ether (TAME) -
* Acute Toxicity to Daphnids (Daphnia magna) Under Flow-through Conditions.
* Toxicology Report Number 408. Springborn Laboratories, Inc. SLI Report
* 92-12-4545.
F020 258729
EOR
F002 482
F010 4.2
F004 1
F005 RL
F006 Guideline study that followed GLP.
F007 Guideline study that followed GLP.
F020 258728
EOR
F002 482
F010 4.2
F004 1
F005 RM
F006 Statistics: The EC50 was estimated by nonlinear interpolation and 95%
* confidence intervals were calculated by bionomial probability.

F007 Statistics: The EC50 was estimated by nonlinear interpolation and 95%
*   confidence intervals were calculated by bionomial probability.
F020 258725
EOR
F002 482
F010 4.2
F004 1
F005 RS
F006 6-hour LC50 = >120 mg/L based on mean measured values.
**   24-hour LC50 = >120 mg/L based on mean measured values.
**   48-hour LC50 = 100 mg/L based on mean measured values.
**   48-hour NOEC = 83 mg/L based on mean measured values.
**
**   After 24-hours of e
F007 6-hour LC50 = >120 mg/L based on mean measured values.
**   24-hour LC50 = >120 mg/L based on mean measured values.
**   48-hour LC50 = 100 mg/L based on mean measured values.
**   48-hour NOEC = 83 mg/L based on mean measured values.
**
**   After 24-hours of exposure, 15% immobilization was observed among dahpnia
*   exposed to the highest mean measured concentration tested (120 mg/L). At
*   test termination (48 hours), 90% immobilization was observed among
*   daphnia exposed to the 120 mg/L treatment level. In addition, sublethal
*   effects, as defined by lethargy, were observed among all of the surviving
*   daphnia exposed to this treatment level. No immobilization or sublethal
*   effects were observed among daphnia exposed to the remaining
*   concentrations tested. The NOEC established during this study was 83
*   mg/L, based on lethargy. 5% immobilization occurred in the control at 48
*   hours. There was no immobilization in the control prior to this sampling
*   point.
**
**   Analytical results:
**   Nominal treatment levels of 690, 410, 250, 150, and 89 mg A.I./L measured
*   120, 83, 55, 28, and 15 78 mg A.I./L, respectively. Both 0- and 48-hour
*   control samples measured <0.40 mg A.I./L. Mean measured concentrations
*   averaged 19% of the nominal concentrations. Coefficients of variation
*   averaged 11% for all mean measured concentrations. The relatively low
*   recovery obtained for the tested treatment levels (mean=19%) is believed
*   due to the volatile nature of the test material and the size of the test
*   vessels.
**
**   Water quality parameter results:
**   Temperature ranged between 19 to 20°C through the 48-hour exposure. The
*   pH was 8.2 in all treatment levels and the control at time 0, and pH
*   ranged between 8.0 to 8.1 in all treatment levels and the control at the
*   24 and 48-hour samplings. Dissolved oxygen ranged from 9.1 to 9.2 mg/L in
*   all treatment levels and the control at time 0, 8.7 to 9.1 mg/L in all
*   treatment levels and the control at time 24, and 8.8 to 9.0 mg/L in all
*   treatment levels and the control at time 48. Total hardness as mg/L of
*   CaCO3 ranged from 170 to 190 in the control and treatment levels at test
*   initiation. Total alkalinity ansmg/L CaCO3 ranged from 110 to 120 in the
*   control and treatment levels at test initiation. Specific conductance was
*   500 umhos/cm in the control and treatment levels at test initiation.
F020 258726
EOR
F002 482
F010 4.2

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F004 1
F005 TS
F006 CAS #994-05-8; tert-amyl methyl ether; 98.8% purity
F007 CAS #994-05-8; tert-amyl methyl ether; 98.8% purity
F020 258727
EOR
F002 482
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
*    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 258730
EOR
F002 482
F010 4.2
F004 2
F005 RE
F006 U.S. Environmental Protection Agency (U.S. EPA) (2000). EPI SuiteTM,
*    Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.
F007 U.S. Environmental Protection Agency (U.S. EPA) (2000). EPI SuiteTM,
*    Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.
F020 258735
EOR
F002 482
F010 4.2
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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 258734
EOR
F002 482
F010 4.2
F004 2
F005 RS
F006 Calculated 48-hr LC50 for Daphnia = 208.4 mg/L
F007 Calculated 48-hr LC50 for Daphnia = 208.4 mg/L
F020 258731
EOR
F002 482
F010 4.2
F004 2
F005 TC
F006 Experimental water solubility, 5468 mg/l @ 20°C (U.S. EPA, 2000), log
* Kow, 1.55 (Huttunen et al., 1997) and melting point, -82.1°C (U.S. EPA,
* 2000) were entered into the program.
** Class: Neutral organics
F007 Experimental water solubility, 5468 mg/l @ 20°C (U.S. EPA, 2000), log
* Kow, 1.55 (Huttunen et al., 1997) and melting point, -82.1°C (U.S. EPA,
* 2000) were entered into the program.
** Class: Neutral organics
F020 258732
EOR
F002 482
F010 4.2
F004 2
F005 TS
F006 CAS #994-05-8; tert-amyl methyl ether
F007 CAS #994-05-8; tert-amyl methyl ether
F020 258733
EOR
F002 482
F010 4.3
F004 1
F005 ME
F006 The test material was known to be volatile and hence testing was
* conducted in completely filled, stopperred test vessels in order to
* minimize possible losses due to volatilization. Following the
* recommendations in published data (Herman et
F007 The test material was known to be volatile and hence testing was
* conducted in completely filled, stopperred test vessels in order to
* minimize possible losses due to volatilization. Following the
* recommendations in published data (Herman et al. 1990. Aquatic toxicology
* 18: 87-100.; Mayer et al. 2000. Environmental Toxicology and Chemistry
* 19: 2551-2556), in order to prevent inhibition of growth due to the
* restriction of gaseous exchange, additional sodium carbonate was added to
* the culture medium to provide a source of carbon dioxide for algal growth.
**
** The range-finding test was conducted at nominal test concentrations of
* 11, 1000, 5000, and 8000 mg/l for 72 hours. Based on the results the

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*    following test concentrations were assigned to the definitive test: 100,
*    200, 400, 800 and 1600 mg/l. At initiation of the test, the culture
*    contained a nominal cell density of 3 E3 cells per ml.
**
**   Temperature was maintained at 23 to 25 degrees C throughout the test. The
*    pH values of the control cultures increased from pH 7.5 at 0 hours to pH
*    8.8 to 8.9 at 72 hours. The test material vessels showed an increase in
*    pH over the 72-hour period following a concentration dependent pattern
*    with the lower test material concentrations exhibiting a greater increase
*    in pH. This effect was considered to be due to there being greater
*    numbers of viable cells in the lower test concentrations and hence
*    greater utilization of carbonate and bicarbonate from
*    photosynthesis/respiration. In all cases, however, the pH shift was less
*    than 1.5 pH unit. No immediate adsorption of the test material to algal
*    cells occurred.
F020 258736
EOR
F002 482
F010 4.3
F004 1
F005 RE
F006 Fortum Oyj (2003). 2-Methoxy-methylbutane (TAME): Algal inhibition test.
*    SafePharm Laboratories. Project No. 1755/003.
F007 Fortum Oyj (2003). 2-Methoxy-methylbutane (TAME): Algal inhibition test.
*    SafePharm Laboratories. Project No. 1755/003.
F020 258741
EOR
F002 482
F010 4.3
F004 1
F005 RL
F006 Guideline study that followed GLP.
F007 Guideline study that followed GLP.
F020 258740
EOR
F002 482
F010 4.3
F004 1
F005 RM
F006 New genus/species name for the organism tested is Pseudokirchneriella
*    subcapitata.
F007 New genus/species name for the organism tested is Pseudokirchneriella
*    subcapitata.
F020 258738
EOR
F002 482
F010 4.3
F004 1
F005 RS
F006 72-hour EbC50 = 230 mg/L based on mean measured values.
**   72-hour ErC50 = 780 mg/L based on mean measured values.
**   72-hour NOEC = 77 mg/L based on mean measured values.
**
**   Results are based on the geometric mean of measured test concentrations.
F007 72-hour EbC50 = 230 mg/L based on mean measured values.
**   72-hour ErC50 = 780 mg/L based on mean measured values.
**   72-hour NOEC = 77 mg/L based on mean measured values.
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**
**   Results are based on the geometric mean of measured test concentrations.
*    Analysis of the test preparations at 0 hours showed the measured
*    concentrations to range from 83 to 100% of nominal values. After 72 hours
*    there was a slight decline in measured concentrations to 69 to 84% of
*    nominal values. Analysis of samples taken from replicate test vessels
*    that had not been opened during the test period gave measured
*    concentrations of 82 to 96% of nominal values. It was therefore
*    considered that the slight decline in measured test concentrations
*    observed in the test vessels that had been opened on a daily basis in
*    order to enable samples to be removed for the determination of algal cell
*    density was the result of losses due volatility.
F020 258737
EOR
F002 482
F010 4.3
F004 1
F005 TS
F006 CAS #994-05-8; tert-amyl methyl ether
F007 CAS #994-05-8; tert-amyl methyl ether
F020 258739
EOR
F002 482
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
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*    regulatory constraints of the Toxic Substances Control Act (TSCA).  It is
*    a pragmatic approach to SAR as opposed to a theoretical approach.
F020 258742
EOR
F002 482
F010 4.3
F004 2
F005 RE
F006 U.S. Environmental Protection Agency (U.S. EPA) (2000). EPI SuiteTM,
*    Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.
F007 U.S. Environmental Protection Agency (U.S. EPA) (2000). EPI SuiteTM,
*    Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.
F020 258747
EOR
F002 482
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 258746
EOR
F002 482
F010 4.3
F004 2
F005 RS
F006 Calculated 96-hr EC50 for a green alga = 126.9 mg/L
**   Calculated 96-hr ChV for a green alga = 9.8 mg/L
F007 Calculated 96-hr EC50 for a green alga = 126.9 mg/L
**   Calculated 96-hr ChV for a green alga = 9.8 mg/L
F020 258743
EOR
F002 482
F010 4.3
F004 2
F005 TC
F006 Experimental water solubility, 5468 mg/l @ 20°C (U.S. EPA, 2000), log
*    Kow, 1.55 (Huttunen et al., 1997) and melting point, -82.1°C (U.S. EPA,
*    2000) were entered into the program.
**   Class: Neutral organics
F007 Experimental water solubility, 5468 mg/l @ 20°C (U.S. EPA, 2000), log
*    Kow, 1.55 (Huttunen et al., 1997) and melting point, -82.1°C (U.S. EPA,
*    2000) were entered into the program.
**   Class: Neutral organics
F020 258744
EOR
F002 482
F010 4.3
F004 2
F005 TS
F006 CAS #994-05-8; tert-amyl methyl ether
F007 CAS #994-05-8; tert-amyl methyl ether
F020 258745
EOR
F002 482
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F010 5.1.1
F004 1
F005 CL
F006 TAME has a low order of toxicity by the oral route of exposure.
F007 TAME has a low order of toxicity by the oral route of exposure.
F020 260337
EOR
F002 482
F010 5.1.1
F004 1
F005 RE
F006 Daughtrey WC and Bird MG (1995). Genotoxicity and twenty-eight-day
* subchronic toxicity studies on tertiary amyl methyl ether. J Applied
* Toxicology 15(4), 313-319.
F007 Daughtrey WC and Bird MG (1995). Genotoxicity and twenty-eight-day
* subchronic toxicity studies on tertiary amyl methyl ether. J Applied
* Toxicology 15(4), 313-319.
F020 258752
EOR
F002 482
F010 5.1.1
F004 1
F005 RM
F006 test type: acute oral toxicity
** route of administration: oral gavage
** dose level: variable
** dose volume: variable
F007 test type: acute oral toxicity
** route of administration: oral gavage
** dose level: variable
** dose volume: variable
F020 258748
EOR
F002 482
F010 5.1.1
F004 1
F005 RS
F006 LD50 ~ 2.1 g/kg (combined sexes)
F007 LD50 ~ 2.1 g/kg (combined sexes)
F020 258750
EOR
F002 482
F010 5.1.2
F004 1
F005 CL
F006 TAME has a low order of toxicity by the inhalation route of exposure.
F007 TAME has a low order of toxicity by the inhalation route of exposure.
F020 258755
EOR
F002 482
F010 5.1.2
F004 1
F005 RE
F006 Amoco (1991). Acute inhalation toxicity study of tert-amyl methyl ether
* (TAME) in rats. Project No. LO8100 1652. IIT Research Institute Life
* Sciences Research, Chicago, IL, USA.
F007 Amoco (1991). Acute inhalation toxicity study of tert-amyl methyl ether

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*    (TAME) in rats.  Project No. LO8100 1652. IIT Research Institute Life
*    Sciences Research, Chicago, IL, USA.
F020 258756
EOR
F002 482
F010 5.1.2
F004 1
F005 RM
F006 Animals were exposed to TAME vapor for 4 hours in a whole body exposure
*    chamber at a concentration of 5.4 mg/L.  TAME concentration was measured
*    by infrared absorption.  Animals were observed for 14 days post exposure.
F007 Animals were exposed to TAME vapor for 4 hours in a whole body exposure
*    chamber at a concentration of 5.4 mg/L.  TAME concentration was measured
*    by infrared absorption.  Animals were observed for 14 days post exposure.
F020 258753
EOR
F002 482
F010 5.1.2
F004 1
F005 RS
F006 There were no premature deaths during the course of the study.
**   During the post-mortem evaluation, seven animals showed external
*    hemorrhagic lung foci, with one female having numerous foci (>10).  One
*    male had a diffused red area on the lu
F007 There were no premature deaths during the course of the study.
**   During the post-mortem evaluation, seven animals showed external
*    hemorrhagic lung foci, with one female having numerous foci (>10).  One
*    male had a diffused red area on the lungs.  Six animals showed enlarged
*    mandibular lymph nodes.  However, the study authors indicated that the
*    observed lung foci were in most cases of a type and number commonly seen
*    in control animals of this strain. LC50 > 5.4 mg/L.
F020 258754
EOR
F002 482
F010 5.1.3
F004 1
F005 CL
F006 TAME was of low dermal toxicity in rats.  LD50 > 3160 mg/kg.
F007 TAME was of low dermal toxicity in rats.  LD50 > 3160 mg/kg.
F020 258761
EOR
F002 482
F010 5.1.3
F004 1
F005 RE
F006 Exxon (1985). Acute dermal toxicity study in the rabbit. Project No.
*    254806. Bio/dynamics Inc., East Laboratory, East Millstone, NJ, USA.
F007 Exxon (1985). Acute dermal toxicity study in the rabbit. Project No.
*    254806. Bio/dynamics Inc., East Laboratory, East Millstone, NJ, USA.
F020 258762
EOR
F002 482
F010 5.1.3
F004 1
F005 RM
F006 TAME was applied neat to the skin of each animal at a dose level of 3160
*    mg/kg.  An occlusive patch covered the test material during the 24 hour
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*    exposure period. Animals were observed for 14 days post exposure.
F007 TAME was applied neat to the skin of each animal at a dose level of 3160
*    mg/kg.  An occlusive patch covered the test material during the 24 hour
*    exposure period. Animals were observed for 14 days post exposure.
F020 258757
EOR
F002 482
F010 5.1.3
F004 1
F005 RS
F006 There were no premature deaths during the study.  However, it was
*    irritating to the skin of the rats.  Very slight to severe erythema and
*    slight to very slight edema were observed in all animals.  Desquamation
*    was seen in all animals on day
F007 There were no premature deaths during the study.  However, it was
*    irritating to the skin of the rats.  Very slight to severe erythema and
*    slight to very slight edema were observed in all animals.  Desquamation
*    was seen in all animals on days 10 and 14; eschar was seen in five
*    animals and atonia in three animals.  One animal showed blanching on day
*    3.  At necropsy, desquamation was noted in two animals and another was
*    considered to be slightly emaciated.
F020 258758
EOR
F002 482
F010 5.3
F004 1
F005 CL
F006 TAME is not a dermal sensitizer
F007 TAME is not a dermal sensitizer
F020 258767
EOR
F002 482
F010 5.3
F004 1
F005 RE
F006 American Petroleum Institute (1995). Closed-patch repeated insult dermal
*    sensitization study of tertiary amyl methyl ether (TAME) in guinea pigs
*    (Buehler Method). Project No. 403. Bio/dynamics Inc., East Laboratory,
*    East Millstone, NJ, USA.
F007 American Petroleum Institute (1995). Closed-patch repeated insult dermal
*    sensitization study of tertiary amyl methyl ether (TAME) in guinea pigs
*    (Buehler Method). Project No. 403. Bio/dynamics Inc., East Laboratory,
*    East Millstone, NJ, USA.
F020 258768
EOR
F002 482
F010 5.3
F004 1
F005 RM
F006 Route of administration:  Dermal
**   Dose volume:  0.3 ml neat
**   Control group included:  Positive and negative controls included
**   Number of animals:  Test group--10/sex; Control group--5/sex
F007 Route of administration:  Dermal
**   Dose volume:  0.3 ml neat
**   Control group included:  Positive and negative controls included
**   Number of animals:  Test group--10/sex; Control group--5/sex
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F020 258763
EOR
F002 482
F010 5.3
F004 1
F005 RS
F006 TAME was non-sensitizing to the skin of guinea pigs
F007 TAME was non-sensitizing to the skin of guinea pigs
F020 258764
EOR
F002 482
F010 5.3
F004 1
F005 TC
F006 During the induction phase (days 1, 8 and 15), TAME (approximately 0.3
* ml) was applied to the clipped area on the back of the test animals for 6
* hours, using an occlusive chamber. Excess material was wiped off at the
* conclusion of each exp
F007 During the induction phase (days 1, 8 and 15), TAME (approximately 0.3
* ml) was applied to the clipped area on the back of the test animals for 6
* hours, using an occlusive chamber. Excess material was wiped off at the
* conclusion of each exposure. The control animals received mineral oil in
* place of the test chemical under similar conditions.
**
** During the challenge phase (day 29), TAME was applied to a clipped area
* on the back which had not previously been exposed for 6 hours, using an
* occlusive chamber; a vehicle control (mineral oil) was also used; a
* further previously untreated group of 5/sex was used as irritation
* control.
F020 258765
EOR
F002 482
F010 5.3
F004 1
F005 TS
F006 Tertiary Amyl Methyl Ether (CAS No. 994-05-8)
** Chemical Name: butane, 2-methoxy-2-methyl-
** Source/purity not specified.
F007 Tertiary Amyl Methyl Ether (CAS No. 994-05-8)
** Chemical Name: butane, 2-methoxy-2-methyl-
** Source/purity not specified.
F020 258766
EOR
F002 482
F010 5.4
F004 1
F005 CL
F006 The NOAEL for subchronic toxicity was 1500 ppm in both males and females.
F007 The NOAEL for subchronic toxicity was 1500 ppm in both males and females.
F020 258773
EOR
F002 482
F010 5.4
F004 1
F005 RE
F006 American Petroleum Institute (1997). A 13-week inhalation
* toxicity/neurotoxicity study of tert-amyl methyl ether (TAME) in the rat

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*    and mouse via whole-body exposures with a 4-week recovery period. Project
*    No. 95-6101. Huntingdon Life Scienc
F007 American Petroleum Institute (1997). A 13-week inhalation
*    toxicity/neurotoxicity study of tert-amyl methyl ether (TAME) in the rat
*    and mouse via whole-body exposures with a 4-week recovery period. Project
*    No. 95-6101. Huntingdon Life Sciences, East Millstone, NJ, USA.
F020 258774
EOR
F002 482
F010 5.4
F004 1
F005 RM
F006 Fischer 344 rats were exposed to 0, 250, 1500 and 3500 ppm TAME for 6
*    hours per day, generally 5 days per week for 13 weeks (minimum 65
*    exposures). Groups of 10/sex at 0 ppm and 3500 ppm were allowed a 4 week
*    recovery period.  A satellite g
F007 Fischer 344 rats were exposed to 0, 250, 1500 and 3500 ppm TAME for 6
*    hours per day, generally 5 days per week for 13 weeks (minimum 65
*    exposures). Groups of 10/sex at 0 ppm and 3500 ppm were allowed a 4 week
*    recovery period.  A satellite group of 10/sex/dose was used for acute
*    neurological testing.
**
**   Animals were observed twice daily for mortality or obvious signs of
*    toxicity, and given a detailed examination each week.  Body weight and
*    food consumption measurements were performed twice pre-test and weekly
*    during the study.  Ophthalmology evaluations were performed pre-exposure,
*    at termination and at the end of the recovery period.  Neurobehavioral
*    studies were performed pre-test and on weeks 2,3,5,9 and 14.  Hematology
*    and serum chemistry evaluations were performed during weeks 5 or 6, week
*    14 and following recovery.  Cell proliferation was assessed in kidney by
*    examination of incorporation of 5-bromo-2'-deoxyuridine after 1, 4 and 13
*    weeks exposure to TAME.  Nephropathy was evaluated by the presence of
*    hyaline droplets, and specific staining for a2µ-globulin in the proximal
*    convoluted tubules.  Animals were subject to a full macroscopic
*    examination at autopsy, and selected organs weighed, sampled and
*    preserved for all animals.  Selected tissues from the control and high
*    dose rats were processed, stained and examined by light microscopy.
F020 258770
EOR
F002 482
F010 5.4
F004 1
F005 RM
F006 Number of animals:  51/sex for the control and high dose groups; 41/sex
*    for the low and mid dose groups
F007 Number of animals:  51/sex for the control and high dose groups; 41/sex
*    for the low and mid dose groups
F020 260355
EOR
F002 482
F010 5.4
F004 1
F005 RS
F006 A number of effects were observed at the highest dose used, 3500 ppm.
*    These included two deaths, post-exposure clinical signs, acute
*    neurological effects, decreased body weight and body weight gain,
*    increased platelet counts, increases in
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F007 A number of effects were observed at the highest dose used, 3500 ppm.
* These included two deaths, post-exposure clinical signs, acute
* neurological effects, decreased body weight and body weight gain,
* increased platelet counts, increases in total protein, albumin and
* globulin, and a number of effects on organ weights. Many of these
* resolved after the 4 week recovery period. There were effects on the
* body weight and brain weight of males after this time. The effects on
* the kidneys of the male rats were consistent with the male rat specific
* a2µ-globulin syndrome and were not considered to be relevant to risk
* assessment in humans.
**
** Exposure of rats at 1500 ppm resulted in effects including post exposure
* clinical signs, acute neurological effects (males only), increased
* platelet count in males, increases in total protein, albumin and globulin
* and effects on liver and kidney (only in females) weight. An increase in
* liver weights of male rats exposed to 250 ppm was also observed. Many of
* these resolved after the 4 week recovery period.
**
** No test material related changes in motor activity were observed at any
* doses. Functional observational battery (FOB) tests were performed on
* the satellite group 1, 6 and 24 hours after acute exposure. Central
* nervous system (CNS) depression, indicated by postural changes, drooping
* or half-closed eyelids, slight stupor or lack of reflex responses, and
* lack of neuromuscular coordination, indicated by ataxia, impaired
* locomotion, poor righting reflex, reduced grip strength and increased
* landing foot splay, were seen in most 3500 ppm animals and a few 1500 ppm
* males after 1 hour. After 6 hours, one 3500 ppm male was in a low
* arousal state and a slight decrease in hindlimb grip strength in the 3500
* ppm females was observed. After 24 hours, the FOB test results for all
* groups were comparable to controls.
**
** Following repeated exposures for a second satellite group of 10/sex/dose,
* an increase in forelimb grip strength was recorded in the 3500 ppm males
* and 1500 and 3500 ppm females. No other effects on measures of
* neuromuscular function or CNS depression were observed.
**
** Microscopic examination of the brain, spinal cord (cervical, thoracic,
* lumbar) and sciatic, sural and tibial nerves showed no evidence of any
* treatment-related effects.
**
** The increased severity of hypertrophy/hyperplasia of the goblet cells in
* the respiratory mucosa and in the epithelium lining the nasopharynx was
* observed in the 3500 ppm group. This effect was considered to be a
* localized adaptive response to a minimal irritant effects rather than an
* adverse toxicological response to the test material. Similar responses
* have been seen in rats exposed to mild irritants such as cigarette smoke,
* formaldehyde, and ammonia.
F020 258771
EOR
F002 482
F010 5.4
F004 2
F005 CL
F006 The NOAEL for subchronic toxicity was 1500 ppm in both males and females.
F007 The NOAEL for subchronic toxicity was 1500 ppm in both males and females.
F020 258779
EOR

F002 482
F010 5.4
F004 2
F005 RE
F006 American Petroleum Institute (1997). A 13-week inhalation
*   toxicity/neurotoxicity study of tert-amyl methyl ether (TAME) in the rat
*   and mouse via whole-body exposures with a 4-week recovery period. Project
*   No. 95-6101. Huntingdon Life Scienc
F007 American Petroleum Institute (1997). A 13-week inhalation
*   toxicity/neurotoxicity study of tert-amyl methyl ether (TAME) in the rat
*   and mouse via whole-body exposures with a 4-week recovery period. Project
*   No. 95-6101. Huntingdon Life Sciences, East Millstone, NJ, USA.
F020 258780
EOR
F002 482
F010 5.4
F004 2
F005 RM
F006 CD-1 mice were exposed to 0, 250, 1500 and 3500 ppm TAME initially; a new
*   high dose group of mice at 2500 ppm and corresponding control group were
*   established due to high mortality at 3500 ppm. Exposures were for 6
*   hours per day, generally
F007 CD-1 mice were exposed to 0, 250, 1500 and 3500 ppm TAME initially; a new
*   high dose group of mice at 2500 ppm and corresponding control group were
*   established due to high mortality at 3500 ppm. Exposures were for 6
*   hours per day, generally 5 days per week for 13 weeks (minimum 65
*   exposures); groups of 10/sex at 0 ppm and the highest dose, 2500 ppm were
*   allowed a 4 week recovery period.
**
**   Animals were observed twice daily for mortality or obvious signs of
*   toxicity, and given a detailed examination each week. Body weight and
*   food consumption measurements were performed twice pre-test and weekly
*   during the study. Ophthalmology evaluations were performed pre-exposure,
*   at termination and at the end of the recovery period.   Hematology and
*   serum chemistry evaluations were performed during weeks 5 or 6, week 14
*   and following recovery. Cell proliferation was assessed in liver by
*   examination of incorporation of 5-bromo-2'-deoxyuridine after 1, 4 and 13
*   weeks exposure to TAME. Animals were subject to a full macroscopic
*   examination at autopsy, and selected organs weighed, sampled and
*   preserved for all animals. Selected tissues from the control and high
*   dose rats were processed, stained and examined by light microscopy.
F020 258776
EOR
F002 482
F010 5.4
F004 2
F005 RM
F006 Number of animals: 46/sex for the control and high dose groups (two
*   groups each); 36/sex for the low and mid dose groups
F007 Number of animals: 46/sex for the control and high dose groups (two
*   groups each); 36/sex for the low and mid dose groups
F020 260356
EOR
F002 482
F010 5.4
F004 2
F005 RS

F006 At 3500 ppm, 13 of 46 males and 10 of 46 females died after the first
* exposure and 26 of 46 males and 14 of 46 females died within three
* exposures to TAME. A trial was conducted with groups of 15 mice/sex
* exposed at 3000 ppm; 8 males and 4
F007 At 3500 ppm, 13 of 46 males and 10 of 46 females died after the first
* exposure and 26 of 46 males and 14 of 46 females died within three
* exposures to TAME. A trial was conducted with groups of 15 mice/sex
* exposed at 3000 ppm; 8 males and 4 females died within eight exposures.
* Accordingly the high dose was set at 2500 ppm.
**
** A number of effects were observed at the highest dose used in the main
* study, 2500 ppm. These included 27 deaths among 92 mice, post-exposure
* clinical signs, effects on a number of clinical chemistry parameters, and
* increased liver weights. Many of these resolved after the 4 week recovery
* period. Liver cell proliferation studies showed increases in the
* labelling index of hepatocytes and centrilobular hepatocellular
* hypertrophy was observed in both sexes.
**
** Exposure of mice at 1500 ppm resulted in effects including post exposure
* clinical signs, increased globulin in males at week 6 and effects on
* liver weights in males. Similar findings were made in the liver cell
* proliferation studies and microscopic examination to those for the 2500
* ppm animals. These liver effects were also observed for female mice
* exposed to 250 ppm.
**
** Centrilobular hepatocellular hypertrophy is frequently seen in the liver
* following exposure to agents that cause hepatic enzyme induction.
* Therefore, this effect is considered an adaptive response to increased
* metabolic load.
F020 258777
EOR
F002 482
F010 5.4
F004 3
F005 CL
F006 The NOAEL for subchronic toxicity was 500 ppm in both males and females.
F007 The NOAEL for subchronic toxicity was 500 ppm in both males and females.
F020 260340
EOR
F002 482
F010 5.4
F004 3
F005 RE
F006 White RD, Daughtrey, WC, Wells, MS (1995). Health effects of inhaled
* tertiary amyl methyl ether and ethyl tertiary butyl ether. Toxicol Lett
* 82/83, 719-724.
F007 White RD, Daughtrey, WC, Wells, MS (1995). Health effects of inhaled
* tertiary amyl methyl ether and ethyl tertiary butyl ether. Toxicol Lett
* 82/83, 719-724.
F020 260341
EOR
F002 482
F010 5.4
F004 3
F005 RM
F006 Number of animals: 14/sex/dose group
F007 Number of animals: 14/sex/dose group

F020 260353
EOR
F002 482
F010 5.4
F004 3
F005 RM
F006 Sprague-Dawley rats were exposed to 0, 500, 2000 and 4000 ppm TAME for 6
*   hours per day, 5 days per week for 4 weeks. Animals were observed at
*   least once daily for mortality or obvious signs of toxicity. Body
*   weights were measured at the i
F007 Sprague-Dawley rats were exposed to 0, 500, 2000 and 4000 ppm TAME for 6
*   hours per day, 5 days per week for 4 weeks. Animals were observed at
*   least once daily for mortality or obvious signs of toxicity. Body
*   weights were measured at the initiation of the study, weekly during the
*   exposure, and immediately before termination of the animal. All rats
*   were fasted for approximately 18 hours following the final exposure to
*   TAME and anesthetized with sodium pentobarbital. Blood samples were
*   obtained for serum chemistry and hematology parameters.
**
**   In addition to daily observation for general toxicity, the study included
*   a functional observational battery (FOB) to evaluate neuromuscular
*   function and sensory perception. The FOB was performed 1 week prior to
*   the first exposure and after 1, 5, or 20 exposures. Four TAME-exposed
*   animals were evaluated approximately 1 hour after the end of exposure and
*   10 animals were examined the following morning in each exposure group.
*   The FOB consisted of an evaluation of the following parameters: tail
*   pinch, rotorod performance, body temperature, righting reflex, auditory
*   response, hindlimb extension, foot splay, grip strength, home-cage
*   observation, hand-held observation, open-field observation, extensor
*   thrust, catalepsy, visual placing, tactile placing, negative geotaxis,
*   vision, eyeblink, and pupil response.
**
**   Necropsies were performed on 10 of the TAME-exposed rats. The following
*   tissues were weighed and fixed in 10% neutral buffered formalin: brain,
*   adrenal glands, gonads, heart, kidneys, liver, lungs and spleen.
*   Approximately 31 other tissues were also collected and fixed at necropsy.
*   Only those from the high exposure and control groups were processed for
*   histological examination.
**
**   For all quantitative parameters, the data were analyzed using both
*   multivariate and univariate two-factor fixed-effects analyses of
*   variance. Quantal data for functional observational battery (FOB)
*   parameters were analyzed using chi-square. A minimum significance level
*   of P<0.05 was used in all comparisons.
F020 260338
EOR
F002 482
F010 5.4
F004 3
F005 RS
F006 Three out of 14 males and 4 out of 14 females exposed to 4000 ppm TAME
*   died on test. The deaths were apparently due to severe central nervous
*   system (CNS) depression as there were no gross or histopathology changes
*   to indicate organ-specif
F007 Three out of 14 males and 4 out of 14 females exposed to 4000 ppm TAME
*   died on test. The deaths were apparently due to severe central nervous
*   system (CNS) depression as there were no gross or histopathology changes

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*    to indicate organ-specific tissue injury.
**
**   Clinical observations in both the 2000 and 4000 ppm TAME-exposed groups
*    included sedation, coma, ataxia, coldness to touch, ptosis,
*    hyperirritability, hypoactivity and effects on posture.  The incidence
*    and severity of effects were greater in the high dose animals.  The FOB
*    assessment confirmed the clinical observations.  TAME-exposed animals
*    evaluated 1 hour after exposure, especially the 4000 ppm group, displayed
*    reductions in tail pinch response, righting reflex and negative geotaxis,
*    along with reduced body temperature, impaired rotorod performance and
*    increased hindlimb splay.  The signs of CNS depression were absent in
*    animals examined 18 hours after the end of exposure. .
**
**   Body weight gain was significantly reduced only in male rats exposed to
*    4000 ppm TAME.  Exposure to 2000 and 4000 ppm TAME caused an increase in
*    relative liver weights in males and females.  Many relative organ weights
*    were increased for the 4000 ppm males due to the reduced body weights of
*    these animals.
**
**   No treatment-related histopathological findings were noted.  Clinical
*    chemistry and hematology findings were minimal with TAME.  Increased
*    serum cholesterol was found in both male rats (at 2000 and 4000 ppm) and
*    female rats (at 4000 ppm) exposed to TAME.  The 4000 ppm males also had
*    reduced serum triglycerides.  A single male rat in the 4000 ppm group had
*    an increase in serum alanine aminotransferase (ALT).  This animal also
*    displayed multifocal hepatocellular necrosis that can be associated with
*    elevated ALT.  The significance of this finding is unclear as this
*    occurred in only one of the seven animals examined. (Three animals had
*    died on test due to CNS depression.)
F020 260339
EOR
F002 482
F010 5.4
F004 4
F005 CL
F006 The NOAEL for subchronic toxicity was 500 mg/kg/day in both males and
*    females.
F007 The NOAEL for subchronic toxicity was 500 mg/kg/day in both males and
*    females.
F020 260344
EOR
F002 482
F010 5.4
F004 4
F005 RE
F006 Daughtrey WC and Bird MG (1995). Genotoxicity and twenty-eight-day
*    subchronic toxicity studies on tertiary amyl methyl ether. J Applied
*    Toxicology 15(4), 313-319.
F007 Daughtrey WC and Bird MG (1995). Genotoxicity and twenty-eight-day
*    subchronic toxicity studies on tertiary amyl methyl ether. J Applied
*    Toxicology 15(4), 313-319.
F020 260345
EOR
F002 482
F010 5.4
F004 4
F005 RM
```

F006 Number of animals: 5/sex/dose group
F007 Number of animals: 5/sex/dose group
F020 260354
EOR
F002 482
F010 5.4
F004 4
F005 RM
F006 Sprague-Dawley rats were exposed to 0, 125, 500 and 1000 mg/kg/day TAME
*   in corn oil by gavage at a dose volume of 2 ml/kg. Vehicle control
*   animals received corn oil only. The dosing regimen was once daily, 7
*   days a week for a period of 29
F007 Sprague-Dawley rats were exposed to 0, 125, 500 and 1000 mg/kg/day TAME
*   in corn oil by gavage at a dose volume of 2 ml/kg. Vehicle control
*   animals received corn oil only. The dosing regimen was once daily, 7
*   days a week for a period of 29 days.
**
**   Observations were made daily for overt signs of toxicity. Body weights
*   were recorded prior to the first dosing and weekly thereafter during the
*   test period. Food consumption was measured weekly over the course of the
*   study. At study termination, blood samples were collected from all
*   animals (after an overnight fast) for routine hematology and serum
*   chemistry determinations. A complete necropsy was carried out on all
*   animals, and organ weights were obtained for the kidneys, adrenals,
*   liver, testes and ovaries. The following tissues were preserved in 10%
*   neutral buffered formalin: kidneys, adrenals, liver, heart, spleen,
*   ovaries, testes and any tissues appearing abnormal. All tissues
*   preserved from the control and high-dose group, as well as those from
*   animals that died during the study, were processed, sectioned, stained
*   with hematoxylin and eosin and examined microscopically.
**
**   Data from the treated groups were compared to those of the control group
*   using the following tests. Comparisons were limited to within-sex
*   analysis. Bartlett's test of homogeneity of variance was used to
*   determine if the groups had equivalent variance at the 1% level. If the
*   variances were not statistically different, the groups were compared
*   using a standard one-way analysis of variance. If significant
*   differences among the means were indicated, Dunnett's test was used to
*   determine which treatment groups differed from controls. Where groups
*   did not have equivalent variance, the non-parametric Kruskall-Wallis test
*   was used to assess differences in group means. If the means were
*   different, Dunn's summed rank test was used to determine which treatment
*   group differed from control.
F020 260342
EOR
F002 482
F010 5.4
F004 4
F005 RS
F006 Four animals (two males, two females) in the high-dose (1000 mg/kg/day)
*   group died during the course of the study. Of these four, two deaths
*   were attributed to dosing accidents. The remaining two deaths were
*   presumed to be test-material r
F007 Four animals (two males, two females) in the high-dose (1000 mg/kg/day)
*   group died during the course of the study. Of these four, two deaths
*   were attributed to dosing accidents. The remaining two deaths were
*   presumed to be test-material related, although a precise cause of death

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*    could not be identified.  All other animals survived to the scheduled
*    termination.
**
**   For the most part, in-life observations were unremarkable.  Lung rales
*    and anogenital staining of the fur were observed at a low frequency in
*    the high-dose group.  The majority of animals of either sex did not
*    exhibit any unusual symptoms or behaviors.
**
**   Overall increases in body weight were noted for all groups of animals.
*    However, mean body weights of high-dose males were significantly lower
*    than those of control males at day 7, day 21 and day 28.  Mean body
*    weight gain in high-dose females was also lower than in control females,
*    although the difference was not statistically significant.  Food
*    consumption in high-dose males and females was also significantly reduced
*    compared to controls during week 1. During week 2, food consumption was
*    significantly reduced only in high-dose males.
**
**   A dose-related increase in adrenal weights (absolute and relative
*    weights) was observed that was statistically significant in the mid- and
*    high-dose males.  A similar increase in adrenal weights was not observed
*    in female rats dosed with TAME.  Relative kidney weights were also
*    increased in mid- and high-dose male rats compared to control.
**
**   Hematology and serum chemistry values were generally similar across
*    groups.  Activated partial thromboplastin time was statistically
*    increased in the high-dose male (but not female) group.  However, this
*    small increase was not believed to be biologically meaningful.  The mean
*    serum glucose value was also significantly reduced in the high-dose male
*    group.  The biological significance of this finding was unknown, however
*    a similar decrease in serum glucose was not observed in high-dose females.
**
**   No treatment-related tissue lesions were observed during the
*    histopathological examination.  Any changes observed were limited to
*    naturally occurring lesions that were present in approximately equal
*    frequency in all groups, including controls.  It was noteworthy that the
*    organ weight increases observed in the kidney and adrenals were not
*    accompanied by any histopathological changes.
F020 260343
EOR
F002 482
F010 5.5
F004 1
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 258784
EOR
F002 482
F010 5.5
F004 1
F005 RE
F006 Daughtrey WC and Bird MG (1995). Genotoxicity and twenty-eight-day
*    subchronic toxicity studies on tertiary amyl methyl ether. J Applied
*    Toxicology 15(4), 313-319.
F007 Daughtrey WC and Bird MG (1995). Genotoxicity and twenty-eight-day
*    subchronic toxicity studies on tertiary amyl methyl ether. J Applied
*    Toxicology 15(4), 313-319.
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F020 258785
EOR
F002 482
F010 5.5
F004 1
F005 RM
F006 Strains tested: Salmonella typhimurium tester strains TA98, TA100,
*   TA1535, TA1537, TA1538
**
**   Test substance doses/concentration levels: The concentration of TAME
*   ranged from 100 to 10,000 ug per plate
**
**   Metabolic activation: With and withou
F007 Strains tested: Salmonella typhimurium tester strains TA98, TA100,
*   TA1535, TA1537, TA1538
**
**   Test substance doses/concentration levels: The concentration of TAME
*   ranged from 100 to 10,000 ug per plate
**
**   Metabolic activation: With and without (S9 fraction mix of livers of
*   Aroclor 1254 pretreated rats)
**
**   Vehicle: Dimethyl sulfoxide (DMSO)
**
**   Positive Controls: 2-aminoanthracene (5 ug/plate); 9-aminoacridine (100
*   ug/plate); N-methyl-N-nitro-N-nitrosoguanidine (MNNG) (10 ug/plate) and
*   2-nitrofluorene (5 ug/plate).
**
**   Statistical analysis: Mean revertant colony count (means of triplicate
*   plates) were determined for each dose point.
**
**   Cytotoxicity study: A toxicity screening test conducted prior to the
*   full assay indicated a lack of toxicity at concentrations as high as
*   10,000 ug per plate.
F020 258781
EOR
F002 482
F010 5.5
F004 1
F005 RS
F006 TAME did not induce reverse gene mutation in any strain. The test
*   substance was not genotoxic in this assay with or without metabolic
*   activation. A satisfactory response was obtained with the positive
*   control substances (2-aminoanthracene,
F007 TAME did not induce reverse gene mutation in any strain. The test
*   substance was not genotoxic in this assay with or without metabolic
*   activation. A satisfactory response was obtained with the positive
*   control substances (2-aminoanthracene, 9-aminoacridine, MNNG,
*   2-nitrofluorene).
F020 258782
EOR
F002 482
F010 5.5
F004 2
F005 CL
F006 TAME was clastogenic under the conditions of this test.
F007 TAME was clastogenic under the conditions of this test.

F020 258790
EOR
F002 482
F010 5.5
F004 2
F005 RE
F006 American Petroleum Institute (1997). Chromosome aberrations in Chinese
* hamster ovary (CHO) cells: Tertiary amyl methyl ether (TAME). Project No.
* G96CJ24.330. Microbiological Associates, Inc., Rockville, MD, USA.
F007 American Petroleum Institute (1997). Chromosome aberrations in Chinese
* hamster ovary (CHO) cells: Tertiary amyl methyl ether (TAME). Project No.
* G96CJ24.330. Microbiological Associates, Inc., Rockville, MD, USA.
F020 258791
EOR
F002 482
F010 5.5
F004 2
F005 RM
F006 Metabolic activation: With and without rat liver S9 from animals
* pretreated with Arochlor 1254
**
** Test type: Chromosome damage
**
** CHO cells were treated with 313, 625, 1250 and 5000 ug/ml TAME in the
* presence and absence of rat liver S9. Ce
F007 Metabolic activation: With and without rat liver S9 from animals
* pretreated with Arochlor 1254
**
** Test type: Chromosome damage
**
** CHO cells were treated with 313, 625, 1250 and 5000 ug/ml TAME in the
* presence and absence of rat liver S9. Cells were treated with TAME for
* 12 hours in the absence of S9 (-S9) and for 4 hours with a 16 hour
* recovery period in the presence of S9. Mitomycin C was used as the
* positive control for experiments conducted in the absence of S9 whereas
* cyclophosphamide was used as the positive control for experiments
* conducted in the presence of S9. Ethanol was the negative control in all
* experiments.
**
** Colcemid (0.1 ug/ml) was added 2 hours before harvest to arrest cells in
* metaphase. TAME was soluble in the treatment medium at all doses tested.
**
** In the absence of S9, a statistically significant increase in aberrant
* cells was observed at 2500 and 5000 ug/ml, and a dose response was
* observed. In the presence of S9, a statistically significant increase in
* aberrant cells was observed at all concentrations and a dose response was
* observed.
**
** The positive controls caused large, statistically significant increases
* in the proportion of aberrant cells in all cases, indicating that the
* test system responded appropriately.
F020 258787
EOR
F002 482
F010 5.6
F004 1
F005 CL

F006 TAME did not produce clastogenic effects in mouse bone marrow.
F007 TAME did not produce clastogenic effects in mouse bone marrow.
F020 258796
EOR
F002 482
F010 5.6
F004 1
F005 RE
F006 Daughtrey WC and Bird MG (1995). Genotoxicity and twenty-eight-day
* subchronic toxicity studies on tertiary amyl methyl ether. J Applied
* Toxicology 15(4), 313-319.
F007 Daughtrey WC and Bird MG (1995). Genotoxicity and twenty-eight-day
* subchronic toxicity studies on tertiary amyl methyl ether. J Applied
* Toxicology 15(4), 313-319.
F020 258797
EOR
F002 482
F010 5.6
F004 1
F005 RM
F006 Tertiary amyl methyl ether was diluted in corn oil and administered as a
* single intraperitoneal (i.p.) injection at doses of 0.75, 0.375 and 0.15
* g/kg body weight. Cyclophosphamide was dissolved in water and used as
* the positive control at
F007 Tertiary amyl methyl ether was diluted in corn oil and administered as a
* single intraperitoneal (i.p.) injection at doses of 0.75, 0.375 and 0.15
* g/kg body weight. Cyclophosphamide was dissolved in water and used as
* the positive control at a dose of 40 mg/kg i.p.
**
** Animals from the appropriate groups were euthanized by CO2 at ca. 24, 48
* and 72 hours after administration of test article. Animals dosed with
* cyclophosphamide were taken at 24 hours only. Each group consisted of 10
* animals (five per sex) per time point. At death, both femurs from each
* animal were removed and bone marrow was recovered and suspended in fetal
* bovine serum. Following centrifugation to pellet the tissue, the
* supernatant was drawn off, the pellet resuspended and the suspension
* spread on slides and dried (two slides were prepared per animal). Prior
* to microscopic evaluation, the slides were stained using acridine orange.
**
** One thousand polychromatic erythrocytes from each animal were examined
* for micronuclei formation. Criteria for scoring micronuclei were those
* of Schmid. In addition, the ratio of polychromatic erythrocytes (PCEs)
* to normochromatic erythrocytes (NCEs) was determined by counting 1000
* erythrocytes (PCEs and NCEs). The data were evaluated statistically
* using ANOVA.
F020 260346
EOR
F002 482
F010 5.6
F004 1
F005 RS
F006 All mice survived to scheduled termination. No increase in micronucleus
* frequency was observed at any dose level of TAME or at any of the bone
* marrow collection times. The positive control (cyclophosphamide)
* produced statistically signifi
F007 All mice survived to scheduled termination. No increase in micronucleus
* frequency was observed at any dose level of TAME or at any of the bone

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*    marrow collection times.  The positive control (cyclophosphamide)
*    produced statistically significant increases in micronucleus frequencies
*    in both males and females.  Overt marow toxicity, as measured by a
*    statistically significant decrease in the percentage of polychromatic
*    erythrocytes, was not observed in any of the groups dosed with TAME.  The
*    percentages of polychromatic erythrocytes observed were within the normal
*    range.  Thus, these data indicated that TAME did not cause clastogenic
*    effects in mouse bone marrow.
F020 258793
EOR
F002 482
F010 5.8.1
F004 1
F005 CL
F006 Exposure to TAME vapor for 6 hr/day, 5-7 days/week for two generations,
*    one litter per generation, at 0, 250, 1500 and 3000 ppm resulted in
*    systemic effects at 1500 and 3000 ppm, minimum adult reproductive
*    toxicity at 3000 ppm and offspring
F007 Exposure to TAME vapor for 6 hr/day, 5-7 days/week for two generations,
*    one litter per generation, at 0, 250, 1500 and 3000 ppm resulted in
*    systemic effects at 1500 and 3000 ppm, minimum adult reproductive
*    toxicity at 3000 ppm and offspring toxicity at 1500 and 3000 ppm. The
*    NOAEL for adult reproductive toxicity was 1500 ppm for males and 3000 ppm
*    for females. The NOAEL for offspring toxicity was 250 ppm in rats under
*    the conditions of this study.
F020 260359
EOR
F002 482
F010 5.8.1
F004 1
F005 RE
F006 Tyl RW, Myers CB, Marr MC, Fail PA, Seely JC, Elswick B, James A and
*    Welsch F (2003). Two-generation reproductive toxicity study of inhaled
*    tertiary amyl methyl ether (TAME) vapor in CD® rats. J Appl Toxicol
*    23(6), 397-410.
F007 Tyl RW, Myers CB, Marr MC, Fail PA, Seely JC, Elswick B, James A and
*    Welsch F (2003). Two-generation reproductive toxicity study of inhaled
*    tertiary amyl methyl ether (TAME) vapor in CD® rats. J Appl Toxicol
*    23(6), 397-410.
F020 260360
EOR
F002 482
F010 5.8.1
F004 1
F005 RM
F006 The study began with 30 males and 30 females per group to yield at least
*    20 pregnant females per group at or near term. Exposure began for all F0
*    animals when they were ca. 7 weeks old. Animals were assigned to groups
*    by means of randomizat
F007 The study began with 30 males and 30 females per group to yield at least
*    20 pregnant females per group at or near term. Exposure began for all F0
*    animals when they were ca. 7 weeks old. Animals were assigned to groups
*    by means of randomization stratified by body weight, such that the body
*    weights by gender of all groups were homogeneous by statistical analysis
*    at study initiation.
**
**   The study was conducted with three treatment groups and an air (vehicle
```

control) group, each comprising 30 rats/gender. The target exposure concentrations were 250, 1500 and 3000 ppm. The F0 animals (parents of the F1 generation) and selected F1 offspring (parents of F2 generation) were exposed to TAME vapor for 6 hr/day, 5 days/week, during the premating exposure periods (for at least 10 weeks) and the postmating holding period (males, for ca. 30 days). During mating (both genders), gestation (dams) and lactation (dams) of F1 and F2 litters, exposures were 6 hr/day, 7 days/week. Pregnant dams were not exposed beginning on gestational day (gd) 20. Dams with litters were not exposed on postnatal day (pnd) 0 (day of parturition) through to pnd 4. Exposures to the dams resumed on pnd 5. Retained postwean F2 offspring were not exposed to TAME vapor.

Observations for mortality were made twice daily and clinical examinations were conducted and recorded daily, prior to and after each exposure period, through the course of the study. The body weights of male rats were recorded initially and weekly through mating. The body weights of female rats were recorded in the same manner until confirmation of mating. Females were weighed and the feed consumption was recorded on gd 0, 7, 14 and 20 and on pnd 0, 4, 7, 14, 21 and 28. For the last three weeks of the premating exposure period, vaginal smears were taken for all F0 and F1 females. The slides from the premating period were evaluated for estrous cyclicity and normality. Vaginal smears were taken daily during the 14-day mating period or until mating was confirmed. The observation of vaginal sperm or copulation plug was considered evidence of successful mating.

All pups (F1 and F2 litters) were counted, weighed, sexed and examined as soon as possible after birth to determine the number of viable and stillborn members of each litter. Thereafter, all live pups were counted, their gender determined, weighed individually and examined grossly, and litters were evaluated for survival on pnd 4, 7, 14 and 21 and at weaning (pnd 28).

Statistical method:

The unit of comparison was the male, the female, the pregnant female or litter, as appropriate. Quantitative continuous data (e.g. parental and pup body weights, organ weights, F2 anogenital distance, feed consumption, food efficiency, etc.) were compared among the three treatment groups and the one vehicle control group by the use of Bartlett's test for homogeneitiy of variances. If Bartlett's test indicated a lack of homogeneity of variances (i.e. $P<0.001$), then non-parametric statistical tests were employed for the continuous variables. Non-parametric tests, used for continuous data that did not have homogeneous variances, included the Kruskal-Wallis test to determine whether significant differences were present among the groups, followed by the Mann-Whitney U test for pairwise comparisons to the vehicle control group if the Kruskal-Wallis test was significant. Jonckheere's test for k independent samples was used to identify significant dose-response trends for non-parametric continous data. If Bartlett's test indicated homogeneous variances (i.e. $P>0.001$), then parametric statistical tests were employed for the continuous variables. A general linear model (GLM) procedures for the analysis of variance (ANOVA) were used to determine the significance of the dose-response relationship and to determine whether significant dosage effects had occurred for selected measures. For all statistical tests, the significance limit of 0.05 was used as the criterion for significance. A test for statistical outliers

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*    was performed on parental body weights and feed consumption (in g/day).
*    If examination of pertinent study data did not provide a plausible and
*    biologically sound reason for inclusion of the data flagged as "outlier,"
*    the data were excluded from summarization and analysis and were
*    designated as outliers.  If feed consumption data (in g/ day) were
*    negative for a given animal and period, they were designated
*    "unrealistic" and excluded from summarization and analysis.  If feed
*    consumption data for a given observational interval (e.g. study days 0-7,
*    7-14, 14-28, 28-35, etc.) during the premating exposure period were
*    designated outliers or unrealistic, then summarized data encompassing
*    this period (e.g. study days 0-70 for the premating exposure period) also
*    did not include this value.
F020 260357
EOR
F002 482
F010 5.8.1
F004 1
F005 RS
F006 Adult systemic toxicity was present for F0 and F1 parental animals at
*    1500 and 3000 ppm. At 3000 ppm, there were consistent and persistent
*    reductions in body weights, weight gains and feed consumption (in g/day)
*    in both genders and both gen
F007 Adult systemic toxicity was present for F0 and F1 parental animals at
*    1500 and 3000 ppm. At 3000 ppm, there were consistent and persistent
*    reductions in body weights, weight gains and feed consumption (in g/day)
*    in both genders and both generations. Feed consumption (in g/kg/day) and
*    food efficiency were variable. Clinical observations at 3000 ppm were
*    limited to ataxia (during and immediately after exposures) in most to all
*    animals in both genders and both generations. Body weights during
*    gestation in F1 dams and during lactation in F0 and F1 dams were reduced
*    at 3000 ppm. At 1500 ppm, there were no effects on body weights, feed
*    consumption or food efficiency, but ataxia was present in F0 males and
*    females and lactational weight change was reduced in F1 dams.
**
**   At necropsy, parental absolute and relative liver weights were increased
*    in both genders and generations at 3000 ppm (in F0 males, absolute and
*    relative kidney weights also were increased at 250 and 1500 ppm).
*    Relative (but not absolute) spleen weights also were increased at 3000
*    ppm. Brain weights, absolute or relative, were not consistently affected.
*    There were no treatment-related gross or histopathological findings for
*    any of these organs.
**
**   Reproductive toxicity:
**   Adult reproductive toxicity was minimally present at 3000 ppm in males,
*    expressed as reduced body weights throughout premating and mating and
*    increased relative (but not absolute) testes weights in F0 and F1 males,
*    most likely due to reduced terminal body weights at this concentration,
*    reduced absolute prostate weight in F1 (but not F0) males, reduced
*    epididymal sperm concentration in F1 (but not F0) males and significantly
*    increased percentage of abnormal sperm in F0 (but not in F1) males. At
*    1500 ppm, the percentage of abnormal sperm was increased relative to the
*    concurrent control value in F0 males, but this value was well within the
*    historical control range for this parameter. There were no effects of
*    treatment on mating or survival indices, absolute testes weight, absolute
*    or relative weights of the epididymides or seminal vesicles with
*    coagulating gland, relative prostate weight, percentage of motile or
*    progressively motile sperm, testicular homogenization-resistant spermatid
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*    head counts, daily sperm production or efficiency of daily sperm
*    production. There were also no treatment-related gross or
*    histopathological findings in the reproductive organs in F0 or F1 males.
**
**   In F0 and F1 females there were no effects of treatment on vaginal
*    cyclicity, estrous cycle length, mating, fertility, pregnancy,
*    gestational indices or gestational length.  Cycle length was reduced at
*    1500 ppm but not at 3000 ppm in F1 females, and not in F0 females at any
*    concentration. This is most likely due to biological variation.
*    Gestational length was significantly longer than the concurrent control
*    values at 1500 ppm, with no effects at 3000 ppm in F1 females and no
*    effects in F0 females at any concentration. The values were all well
*    within the historical control range for this parameter. There were also
*    no effects on number of implantation sites per litter, on number of
*    total, live or dead pups per litter on pnd 0 or on the percentage of
*    postimplantation loss per litter (prenatal mortality index). There were
*    also no effects on absolute or relative ovary or uterine weight and no
*    treatment-related gross or histopathological findings in these organs.
**
**   Offspring toxicity:
**   Offspring toxicity was present at 1500 and 3000 ppm. Survival indices
*    were unaffected for F1 offspring throughout lactation (pnd 4, 7, 14, 21
*    and 28) and were unaffected for F2 offspring for pnd 7, 14 and 28. The F2
*    survival indices were significantly reduced at 3000 ppm for pnd 4 and 21.
*    The F1 pup body weights per litter were significantly reduced during
*    lactation at 1500 and 3000 ppm on pnd 4, 7, 14, 21 and 28 (but not on pnd
*    0) and at 250 ppm on pnd 14, 21 and 28 (the last only for males). The F2
*    pup body weights per litter were significantly reduced during lactation
*    at 3000 ppm for pnd 0, 4, 7, 14, 21 and 28 and at 1500 ppm for pnd 14 and
*    21. There were no effects on the F2 pups at 250 ppm.  Delays (not
*    correlated with body weight differences) in the age of preputial
*    separation in males (F1 at 1500 and 3000 ppm, and F2 at 3000 ppm) and
*    vaginal patency in females (F1 at 3000 ppm, and F2 at 250 and 3000 ppm)
*    were observed in both generations. Overall the effects seemed more severe
*    on the F1 generation. Shorter anogenital distances at birth were observed
*    in both sexes of the F2 generation. These appeared to be related to lower
*    birth weights. The pattern exhibited by these results was considered more
*    likely to be due to overall toxicity, rather than endocrine disruption,
*    which would be expected to have more severe effects on one sex than the
*    other.
F020 260358
EOR
F002 482
F010 5.8.2
F004 1
F005 CL
F006 There was no evidence of treatment-related teratogenicity at any of the
*    three exposure concentrations and no other developmental effects.  Almost
*    all the fetal malformation and variation findings were those commonly
*    observed in historical c
F007 There was no evidence of treatment-related teratogenicity at any of the
*    three exposure concentrations and no other developmental effects.  Almost
*    all the fetal malformation and variation findings were those commonly
*    observed in historical control Sprague-Dawley rat fetuses and in
*    published control databases.  Therefore, the NOAEL was 250 ppm for
*    maternal toxicity and 1500 ppm for developmental toxicity in rats under
*    the conditions of this study.
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F020 258802
EOR
F002 482
F010 5.8.2
F004 1
F005 RE
F006 Welsch F, Elswick B, James RA, Marr MC, Myers CB and Tyl RW (2003).
*   Developmental toxicity evaluation of inhaled tertiary amyl methyl ether
*   in mice and rats. J Applied Toxicology 23, 387-395.
F007 Welsch F, Elswick B, James RA, Marr MC, Myers CB and Tyl RW (2003).
*   Developmental toxicity evaluation of inhaled tertiary amyl methyl ether
*   in mice and rats. J Applied Toxicology 23, 387-395.
F020 258803
EOR
F002 482
F010 5.8.2
F004 1
F005 RM
F006 In this study, 25 evidence-of-mating-positive females per group were
*   exposed to TAME for 6 hr/day on 14 consecutive days (gd 6-19). Clinical
*   observations were taken daily, except during the exposure period. During
*   this period they were mad
F007 In this study, 25 evidence-of-mating-positive females per group were
*   exposed to TAME for 6 hr/day on 14 consecutive days (gd 6-19). Clinical
*   observations were taken daily, except during the exposure period. During
*   this period they were made at least twice daily, immediately
**   before and after each daily TAME exposure. Maternal body weights were
*   recorded in the morning on gd 0, 6, 9, 12, 15, 18 and 20. Feed
*   consumption was measured for the intervals gd 0-6, 6-9, 9-12, 12-15,
*   15-18, and 18-20. At scheduled termination on gd 20, the dams were
*   evaluated for body, liver and gravid uterine weights. Ovarian corpora
*   lutea were counted and the status of uterine implantation sites (i.e.
*   resorptions, dead fetuses, live fetuses) was recorded. All fetuses were
*   dissected from the uterus, counted and weighed; their gender was
*   determined and the fetuses were examined for external abnormalities.
*   Approximately half of the fetuses in each litter were examined for
*   visceral malformations and variations by a fresh tissue dissection
*   method. The heads of the fetuses were removed and fixed in Bouin's
*   solution; serial free-hand sections of the heads were examined for
*   soft--tissue craniofacial malformations and variations. All fetuses in
*   each litter were eviscerated, fixed in alcohol and stained with alizarin
*   red S/alcian blue. Intact fetuses (approximately half per litter; the
*   one not examined viscerally or decapitated) were examined for skeletal
*   malformations and variations.
**
**   Statistical method:
**   Quantitative continuous data (e.g. maternal body weights, fetal body
*   weights, maternal feed consumptions, etc.) were compared among the three
*   treatment groups against the air inhalation control group by Bartlett's
*   test for homogeneity of variances. If Bartlett's test indicated lack of
*   homogeneity of variances (i.e. P<0.001), then non-parametric statistical
*   tests were employed for the continuous variables. If Bartlett's test
*   indicated homogeneous variances (i.e. P>0.001), then parametric
*   statistical tests were used. Parametric statistical procedures that were
*   applied to selected measures from this developmental toxicity study were
*   as follows. Appropriate general linear model (GLM) procedures were used
*   for the analysis of variance (ANOVA). Prior to GLM analysis, an arcsine

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*    square root transformation was performed on all litter-derived percentage
*    data to allow the use of parametric methods.  For these litter-derived
*    percentage data, the ANOVA was weighted according to litter size.  The
*    GLM analysis was used to determine the significance of the
*    concentration-response relationship (test for linear trend) and to
*    determine whether significant concentration-related effects had occurred
*    for selected measures (ANOVA).  When a significant (P<0.05) main effect
*    for concentration occurred, Dunnett's multiple comparison test was used
*    to compare each TAME-exposed group to the control group for that measure.
*     A one-tailed
**   Test (i.e. Dunnett's test) was used for all pairwise differences from the
*    air-only control group, except that a two-tailed test was used for
*    maternal body and organ weight parameters, maternal feed consumption,
*    fetal body weight and percent of males per litter.
**   Non-parametric tests were used on continuous data without homogeneous
*    variances and included the Kruskal-Wallis test to determine if
*    significant differences were present among the groups, followed by the
*    Mann-Whitney U test for pairwise differences from the designated control
*    group if the Kruskal-Wallis test was significant. Jonckheere's test for k
*    independent samples was applied to identify significant dose-response
*    trends for non-parametric continuous data.  Nominal scale measures were
*    analyzed by the chi-square test for independence for differences among
*    treatment groups and by the Cochran-Armitage test for a linear trend on
*    proportions.  When the chi-square test revealed significant (P<0.05)
*    differences among groups, a two-tailed Fisher's exact probability test
*    with appropriate adjustment for multiple comparisons was used for
*    pairwise differences between each TAME-exposed group and the control
*    group.  A test for statistical outliers was performed on maternal body
*    weights and feed consumption (in g/day).  If examination of pertinent
*    study data did not provide a plausible and biologically sound reason for
*    inclusion of the data flagged as "outlier," the data were excluded from
*    summarization and analysis and were designated as outliers.  If feed
*    consumption data (in g/day) were negative for a given dam and period,
*    they were designated unrealistic and excluded from summarization and
*    analysis.  If feed consumption data for a given observational interval
*    (e.g. gd 6-9, 9-12, 12-15 or 15-17) were designated outliers or
*    unrealistic, then summarized data encompassing this period (e.g.
*    treatment period) also did not include this value.
F020 258799
EOR
F002 482
F010 5.8.2
F004 1
F005 RS
F006 Maternal toxicity observations:
**
**   Prior to the start of exposures, maternal body weights were equivalent
*    across all groups.  Maternal body weight was significantly reduced only
*    at 3500 ppm for gd 12, 15, 18 and 20 (in-life and at termination
F007 Maternal toxicity observations:
**
**   Prior to the start of exposures, maternal body weights were equivalent
*    across all groups.  Maternal body weight was significantly reduced only
*    at 3500 ppm for gd 12, 15, 18 and 20 (in-life and at termination).
*    Maternal weight change was significantly reduced at 1500 and 3500 ppm for
*    gd 6-9
**   and at 3500 ppm for gd 6-20 (exposure period).  Maternal weight change
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*   was significantly reduced at 1500 and 3500 ppm for gd 0-20 (entire
*   gestation period), as was gestational weight change corrected for weight
*   of the gravid uterus. There were no effects on maternal weight change at
*   250 ppm. Gravid uterine weight exhibited a significant
*   exposure-concentration related downward linear trend (P<0.05) but no
*   statistically significant pairwise comparison differences in any group
*   compared with the concurrent control group. Maternal absolute liver
*   weights were equivalent across all groups. At scheduled necropsy,
*   maternal liver weight relative to body weight was significantly increased
*   at 3500 ppm.
**
**   Maternal feed consumption (in g/day) was significantly reduced at 3500
*   ppm for gd 6-9, 9-12, 12-15, 15-18, 18-20, 6-20 (exposure period) and
*   0-20 (gestation period). At 1500 ppm, feed consumption was significantly
*   reduced only for gd 9-12. When the data were expressed as g/kg/day,
*   maternal feed consumption at 3500 ppm was reduced for gd 6-9, 9-12 and
*   6-20. At 1500 ppm, feed consumption (as g/kg/day) was significantly
*   reduced only for gd 6-9. There were no effects of treatment on maternal
*   feed consumption at 250 ppm.
**
**   Clinical observations related to TAME exposure at 3500 ppm included
*   ataxia (after exposure on gd 6-11), dazed appearance (gd 6-12), lethargy
*   (gd 6-13 and 16-19), eyes squinted (gd 6-8 and 10), eyes closed (gd 8 and
*   11), pica (gd 6-14 and 16), slow respiration (gd 6, 8 and 11),
*   piloerection (gd 6, 7, 9, 15, 16, 17 and 19), rough coat (gd 7, 9 and
*   10), facial tremors (gd 8 and 11), gasping (gd 8) and clinical weight
*   loss (>5.0 g within a weighing period) on gd 9. At 1500 ppm, dams
*   exhibited lethargy (one each on gd 6 and 7) and piloerection (one on gd
*   15). At 250 ppm, one dam exhibited pica on gd 6 and two dams exhibited
*   piloerection on gd 19. There was a clear indication of maternal
*   accommodation to the highest TAME exposure concentration, as evidenced by
*   diminution in incidence and intensity of clinical signs such as ataxia,
*   lethargy and slow respiration over time. At scheduled necropsy, no gross
*   anomalies were found in dams.
**
**   Embryo/fetal toxicity
**
**   There were no significant effects of treatment on gestational parameters,
*   including number of ovarian corpora lutea, total number of uterine
*   implantation sites, pre- or post-implantation loss, number of live
*   fetuses per litter and gender ratio (% male fetuses) per litter. Fetal
*   body weight per litter, when calculated as all fetuses,or males or
*   females separately, was significantly reduced at 3500 ppm.
**
**   There were no treatment-related changes in the incidence of individual or
*   pooled external, visceral, skeletal or total malformation or variations
*   by litter or by fetus per litter. One fetus in one litter at 250 ppm
*   exhibited all the external malformations observed in the TAME-exposed
*   groups of this study: unilateral right anophthalmia, ocular orbits close
*   together, agenesis of the nostril and micrognathia. Fetal visceral
*   malformations were almost exclusively limited to hydronephrosis and
*   hydroureter, distributed across 0. 250 and 1500 ppm, and one fetus in one
*   litter at 0 ppm with interventricular septal defect. For fetal skeletal
*   malformations, one fetus at 0 ppm exhibited fused sternebrae, one fetus
*   at 1500 ppm exhibited scrambled sternebrae and agenesis of a rib and one
*   fetus at 3500 ppm exhibited bipartite cartilage and bipartite
*   ossification center in the thoracic centrum. Fetal external variations

```
*    were distributed across all groups and were limited to hematomas at
*    various locations.  Fetal visceral variations were distributed across all
*    groups with no TAME exposure-related pattern; they included predominantly
*    enlarged laterl ventricles of the cerebrum and distended ureters, both
*    common findings in term fetuses.  Fetal skeletal variations included
*    misaligned sternebrae and changes in cartilage and bone in the thoracic
*    centra, predominantly extra rib (full or rudimentary) on lumbar vertebra
*    no. 1 across all groups examined.  These variations are common fetal
*    findings.
F020 258800
EOR
F002 482
F010 5.8.2
F004 2
F005 CL
F006 TAME caused only unspecific embryotoxic effects that were apparently
*    related to high exposure concentrations and associated concomitant
*    maternal stress. The NOAEL for maternal and developmental toxicity in
*    mice was 250 ppm in the present st
F007 TAME caused only unspecific embryotoxic effects that were apparently
*    related to high exposure concentrations and associated concomitant
*    maternal stress. The NOAEL for maternal and developmental toxicity in
*    mice was 250 ppm in the present study.
F020 258808
EOR
F002 482
F010 5.8.2
F004 2
F005 RE
F006 Welsch F, Elswick B, James RA, Marr MC, Myers CB and Tyl RW (2003).
*    Developmental toxicity evaluation of inhaled tertiary amyl methyl ether
*    in mice and rats. J Applied Toxicology 23, 387-395.
F007 Welsch F, Elswick B, James RA, Marr MC, Myers CB and Tyl RW (2003).
*    Developmental toxicity evaluation of inhaled tertiary amyl methyl ether
*    in mice and rats. J Applied Toxicology 23, 387-395.
F020 258809
EOR
F002 482
F010 5.8.2
F004 2
F005 RM
F006 In this study, 25 evidence-of-mating-positive females per group were
*    exposed to TAME for 6 hrs per day on 11 consecutive days (gd 6-16).
*    Clinical observations were taken daily, except during the exposure
*    period.  During this period they wer
F007 In this study, 25 evidence-of-mating-positive females per group were
*    exposed to TAME for 6 hrs per day on 11 consecutive days (gd 6-16).
*    Clinical observations were taken daily, except during the exposure
*    period.  During this period they were made at least twice daily,
*    immediately
**   before and after each daily TAME exposure.  Maternal body weights were
*    recorded in the morning on gd 0, 6, 9, 12, 15 and 17.  Feed consumption
*    was measured for the intervals gd 0-6, 6-9, 9-12, 12-15, and 15-17.  At
*    scheduled termination on gd 17, the dams were evaluated for body, liver
*    and gravid uterine weights.  Ovarian corpora lutea were counted and the
*    status of uterine implantation sites (i.e. resorptions, dead fetuses,
*    live fetuses) was recorded.  All fetuses were dissected from the uterus,
```

*   counted and weighed; their gender was determined and the fetuses were
*   examined for external abnormalities. Approximately half of the fetuses
*   in each litter were examined for visceral malformations and variations by
*   a fresh tissue dissection method. The heads of the fetuses were removed
*   and fixed in Bouin's solution; serial free-hand sections of the heads
*   were examined for soft--tissue craniofacial malformations and variations.
*   All fetuses in each litter were eviscerated, fixed in alcohol and
*   stained with alizarin red S/alcian blue. Intact fetuses (approximately
*   half per litter; the one not examined viscerally or decapitated) were
*   examined for skeletal malformations and variations.
**
**   Statistical method:
**   Quantitative continuous data (e.g. maternal body weights, fetal body
*   weights, maternal feed consumptions, etc.) were compared among the three
*   treatment groups against the air inhalation control group by Bartlett's
*   test for homogeneity of variances. If Bartlett's test indicated lack of
*   homogeneity of variances (i.e. P<0.001), then non-parametric statistical
*   tests were employed for the continuous variables. If Bartlett's test
*   indicated homogeneous variances (i.e. P>9.001), then parametric
*   statistical tests were used. Parametric statistical procedures that were
*   applied to selected measures from this developmental toxicity study were
*   as follows. Appropriate general linear model (GLM) procedures were used
*   for the analysis of variance (ANOVA). Prior to GLM analysis, an arcsine
*   square root transformation was performed on all liter-derived percentage
*   data to allow the use of parametric methods. For these litter-derived
*   percentage data, the ANOVA was weighted according to litter size. The
*   GLM analysis was used to determine the significance of the
*   concentration-response relationship (test for linear trend) and to
*   determine whether significant concentration-related effects had occurred
*   for selected measures (ANOVA). When a significant (P<0.05) main effect
*   for concentration occurred, Dunnett's multiple comparison test was used
*   to compare each TAME-exposed group to the control group for that measure.
*   A one-tailed
**   Test (i.e. Dunnett's test) was used for all pairwise differences from the
*   air-only control group, except that a two-tailed test was used for
*   maternal body and organ weight parameters, maternal feed consumption,
*   fetal body weight and percent of males per litter.
**   Non-parametric tests were used on continuous data without homogeneous
*   variances and included the Kruskal-Wallis test to determine if
*   significant differences were present among the groups, followed by the
*   Mann-Whitney U test for pairwise differences from the designated control
*   group if the Kruskal-Wallis test was significant. Jonckheere's test for k
*   independent samples was applied to identify significant dose-response
*   trends for non-parametric continuous data. Nominal scale measures were
*   analyzed by the chi-square test for independence for differences among
*   treatment groups and by the Cochran-Armitage test for a linear trend on
*   proportions. When the chi-square test revealed significant (P<0.05)
*   differences among groups, a two-tailed Fisher's exact probability test
*   with appropriate adjustment for multiple comparisons was used for
*   pairwise differences between each TAME-exposed group and the control
*   group. A test for statistical outliers was performed on maternal body
*   weights and feed consumption (in g/day). If examination of pertinent
*   study data did not provide a plausible and biologically sound reason for
*   inclusion of the data flagged as "outlier," the data were excluded from
*   summarization and analysis and were designated as outliers. If feed
*   consumption data (in g/day) were negative for a given dam and period,
*   they were designated unrealistic and excluded from summarization and

```
*    analysis.  If feed consumption data for a given observational interval (
*    e.g. gd 6-9, 9-12, 12-15 or 15-17) were designated outliers or
*    unrealistic, then summarized data encompassing this period (e.g.
*    treatment period) also did not include this value.
F020 258805
EOR
F002 482
F010 5.8.2
F004 2
F005 RS
F006 Maternal toxicity observations:
**
**   In this study, inhalation of TAME by pregnant mice during gestation days
*    6-16 resulted in maternal toxicity at 3500 ppm, including maternal
*    mortality (4 of 25), reductions in body weight, weight gain and tre
F007 Maternal toxicity observations:
**
**   In this study, inhalation of TAME by pregnant mice during gestation days
*    6-16 resulted in maternal toxicity at 3500 ppm, including maternal
*    mortality (4 of 25), reductions in body weight, weight gain and
*    treatment-related clinical signs of toxicity.  The increased maternal
*    absolute and relative liver weights at 1500 and 3500 ppm may have been
*    due to induction of metabolizing enzymes and therefore increase in mass.
**
**   Maternal body weight was significantly reduced only at 3500 ppm for gd 15
*    and 17 (in-life and at termination). Prior to the start of exposures,
*    maternal body weights were equivalent across all groups.  Maternal weight
*    change was significantly reduced at 3500 ppm for gd 9-12, 12-15, 15-17,
*    6-17 (exposure period) and 0-17 (entire gestation period).  Maternal
*    gestational weight change, corrected for the weight of the gravid uterus,
*    was unaffected across groups. There were no effects on maternal weight
*    change at 250 or 1500 ppm.  Gravid uterine weight was significantly
*    reduced at 3500 ppm. Maternal absolute liver weight was significantly
*    increased at 1500 ppm but not at 3500 ppm, although the value at 3500 ppm
*    was slightly increased.  Maternal liver weight relative to weight at
*    termination was significantly increased at 1500 and 3500 ppm.  The
*    increased relative liver weight may also have been due, in part, to the
*    reduced body weights of the dams at termination at 3500 ppm.
**
**   Clinical observations related to TAME exposure at 3500 ppm included
*    ataxia, hyperactivity, prone positioning, lethargy, gasping, rough coat,
*    slow respiration, head tremors, squinted eyes, and maternal mortality. At
*    1500 ppm, dam exhibited half-closed eyes and head tremors.  At 250 ppm,
*    one dam delivered early on gd 16.  In addition to solvent smell on fur,
*    findings for the unscheduled deaths at 3500 ppm included red to dark red
*    nail beds, red foci or red areas on lungs.  These findings appeared to be
*    consistent with severe congestion.  There was clear indication of reduced
*    pharmacological effects with time and maternal accommodation to the top
*    two exposure concentrations.  This interpretation was supported by
*    observations of mortality at 3500 ppm early in the exposure period (gd
*    6-9) only and diminution over time in the incidence of clinical signs of
*    toxicity, such as ataxia, lethargy, gasping and slow respiration. At
*    scheduled necropsy, there were no gross findings in dams indicative of
*    any lesions caused by the TAME exposure.
**
**   Maternal feed consumption (in g/day) was significantly reduced at 3500
*    ppm for gd 9-12, 12-15, 15-17, and 6-17 (exposure period).  Maternal feed
```

* consumption for the gestational period (gd 0-17) was unaffected across
* the other groups. At 1500 ppm, feed consumption was significantly
* reduced only for gd 6-9. When the data were expressed as g/kg/day,
* maternal feed consumption at 3500 ppm reduced only for gd 9-12. At 1500
* ppm, feed consumption (as g/kg/day) was unaffected. There were no
* effects of treatment on maternal feed consumption at 250 ppm.
**
** Embryo/fetal toxicity
**
** There were no significant effects of maternal TAME vapor inhalation on
* gestational parameters, including number of ovarian corpora lutea, total
* number of uterine implantation sites, pre- or post-implantation loss,
* number of live fetuses per litter and gender ratio (% male fetuses) per
* litter. At 3500 ppm, there were significant increases in the percentage
* of late fetal deaths per litter and percentage of litters with late fetal
* deaths. There were significant concentration-related upward trends for
* percentage of non-live implants per litter and percentage of adversely
* affected (non-live plus malformed) implants per litter, with no
* significant pairwise comparisons with the concurrent control group
* values. Fetal body weight per litter when calculated as all fetuses, or
* males or females separately, was significantly reduced at 3500 ppm.
**
** A statistically significant TAME-exposure-related increase was observed
* in the percentage of litters with fetal external malformations at 3500
* ppm (31.68%); the value at 1500 ppm was also increased (18.28%) but not
* statistically significantly relative to the control group value (0.00%).
* A statistically significant, treatment-related increase was also observed
* in the percentage of litters with visceral variations at 3500 ppm
* (89.47%) relative to the control group value (47.83%). Values at 250 ppm
* (52.38%) and 1500 ppm (50.00%) were unchanged from the control group
* value. There were statistically significant, treatment-related upward
* trends (P<0.001) for the percentage of fetuses with variations per litter
* and for the percentage of male fetuses (but not for female fetuses) with
* variations per litter but no significant pairwise comparisons with the
* concurrent control group values for these parameters. The incidences of
* visceral, skeletal and total malformations and of external, skeletal and
* total variations were unchanged across groups when expressed as fetuses
* per litter or as litters with affected fetuses. External malformations
* were limited to cleft palate in three fetuses in three litters at 1500
* ppm and 11 fetuses in six litters at 3500 ppm. One litter at 1500 ppm had
* three fetuses with polydactyly of fore- and hindpaws, one fetus with
* exencephaly and open left eye and one fetus with micrognathia and
* polydactyly. Fetal skeletal malformations were also distributed across
* all groups, with findings limited to the sternum (sternal plate and
* sternebrae) and ribs (branched, fused and inappropriate attachments of
* floating ribs to the sternum).
**
** Fetal external variations were limited to hematomas in various locations
* at 250 and 1500 ppm. Fetal visceral variations were limited mainly to
* enlarged lateral ventricles of the cerebrum across all groups. One fetus
* in one litter at 0 ppm and three fetuses in three litters at 1500 ppm had
* red foci on urinary bladder and one fetus in one litter at 0 ppm had red
* foci on kidney. The incidence of enlarged lateral ventricles (full) and
* bilateral ventricles exhibited a clear treatment-related increased
* incidence only at 3500 ppm, with eight affected fetuses in seven litters
* at 0 ppm, six affected fetuses in four litters at 250 ppm, seven affected
* fetuses in seven litters at 1500 ppm and 38 affected fetuses in 16

```
*    litters at 3500 ppm.  Fetal skeletal variations included extra rib(s) on
*    lumbar vertebra no. 1 in all groups, misaligned sternebrae at 0, 250 and
*    1500 ppm, reduced ossification in sternebrae in all groups, in lumbar
*    centrum at 1500 ppm and in thoracic centrum and pubis at 3500 ppm and
*    floating extra rib cartilage at 1500 ppm.
**
**   Developmental toxicity was present at 3500 ppm, expressed specifically as
*    increased incidence of late fetal deaths, reduced fetal body weights per
*    litter and increased incidences of cleft palate (an external
*    malformation) and of enlarged lateral ventricles of the cerebrum ( a
*    visceral variation).  At 1500 ppm, three fetuses in three litters also
*    exhibited cleft palate (with none observed at 250 of 9 ppm).  This
*    increase was not statistically significant, but it is considered
*    biologically relevant and related to maternal TAME exposure.  The finding
*    of one additional litter at 1500 ppm with three multiply malformed
*    fetuses (out of nine live fetuses total) may be unrelated to treatment
*    because these malformations were not observed at 3500 ppm and were
*    limited to only one litter at 1500 ppm.  The observation of cleft palate
*    in fetuses at 1500 and 3500 ppm appears to be consistent with a proposed
*    mechanism for cleft palate in mice exposed to methyl tertiary butyl ether
*    (MTBE).  Maternal exposure to MTBE with anesthetic qualities at high
*    concentrations associated with maternal stress results in elevated
*    endogenous corticosteroid levels, which cause cleft palate in the
*    developing offspring in mice (Bevan et al., 1997).  Although those
*    hormone levels were not determined in the present study, the biological
*    mode of action of TAME appears to be similar and comparable to that of
*    MTBE, as judged by clinical observations.  At high exposure
*    concentrations in mice, TAME exerts depressant effects on the central
*    nervous system that resemble anesthetic properties and are preceded by a
*    pronounced excitatory stage.  Therefore, the brain stimulation and
*    excitation may have induced a rise in endogenous corticosteroid levels in
*    the mouse dams. The occurrence of a significantly increased incidence of
*    fetal cleft palate at the 3500 ppm exposure level, coincident with
*    maternal toxicity, suggests that stress of the dams is a contributing
*    factor.  Mice are sensitive to stress, and cleft palate occurs in
*    offspring if the pregnant dams experience stress such as food and water
*    deprivation, transportation, restraint or low humidity.  That
*    corticosteroids cause cleft palate in susceptible mouse strains is well
*    documented.
**
**   The increased incidence of enlarged lateral ventricles of the fetal
*    cerebrum at 3500 ppm is consistent with developmental delay because the
*    fetuses at this exposure concentration exhibited mean body weights per
*    litter of ca. 60% of the concurrent control group values.  There were no
*    notable developmental effects at 250 ppm.  Almost all of the fetal
*    malformations and variation findings observed in the present study are
*    documented in control CD-1 mice fetuses collected at the Research
*    Triangle Institute.  In that historical database (47 control mouse
*    litters with 589 fetuses), bilateral enlarged lateral ventricles was the
*    most common fetal visceral variation in control fetuses.
F020 258806
EOB
C
X
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IUCLID

Data Set

Existing Chemical	:	ID: 994-05-8
CAS No.	:	994-05-8
EINECS Name	:	2-Methoxy-2-Methylbutane2-Methoxy-2-Methylbutane
EC No.	:	213-611-4
TSCA Name	:	tert-Amyl Methyl Ether
Molecular Formula	:	C6H14O

Producer related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	28.07.2006

Substance related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	28.07.2006
Status	:	
Memo	:	U.S. EPA - HPV Challenge Program
Printing date	:	01.10.2007
Revision date	:	
Date of last update	:	09.10.2006
Number of pages	:	47
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	**:**	

28.07.2006

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

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	:	= -81.2 °C
Sublimation	:	
Method	:	other: calculated
Year	:	
GLP	:	no data
Test substance	:	other TS: tert-amyl methyl ether (TAME); (CAS #994-05-8) Melting Point is calculated by the MPBPWIN, version 1.41, a subroutine of the computer program EPI SuiteTM, version 3.012, (2000) which is based on the average result of the meth
Method	:	Melting Point is calculated by the MPBPWIN, version 1.41, a subroutine of the computer program EPI SuiteTM, version 3.012, (2000) which is based on the average result of the methods of K. Joback and Gold and Ogle. Joback's Method is described in Joback K (1982). A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. (1987). R Reid, J Prausnitz and B 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 #994-05-8; tert-amyl methyl ether The value was calculated based on chemical structure as modeled by EPI SuiteTM. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

31.07.2006 (22)

2.2 BOILING POINT

Value	:	= 86.3 °C at 1013 hPa
Decomposition	:	
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	other TS: tert-amyl methyl ether (TAME); (CAS #994-05-8)
Test substance	:	CAS #994-05-8; tert-amyl methyl 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

31.07.2006 (17)

2.3 DENSITY

Type	:	density
Value	:	= .7703 g/cm³ at 20 °C
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	other TS: tert-amyl methyl ether (TAME); (CAS #994-05-8)

Test substance	:	CAS #994-05-8; tert-amyl methyl 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

31.07.2006 (17)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	= 90 hPa at 20 °C
Decomposition	:	
Method	:	other (measured)
Year	:	
GLP	:	no data
Test substance	:	other TS: tert-amyl methyl ether (TAME); (CAS #994-05-8)
Method	:	Neste Company method 205 using Grabner apparatus.
Remark	:	Mean of duplicate determinations, SD = 6
Test substance	:	CAS #994-05-8; tert-amyl methyl 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. These data were used for the vapor pressure endpoint in the European Union Risk Assessment for tert-amyl methyl ether (Finnish Environment Institute (2004). 2-Methoxy-Methyl Butane (TAME) Environmental Risk Assessment. Final Draft.).

31.07.2006 (15) (16)

Value	:	= 120 hPa at 25 °C
Decomposition	:	
Method	:	other (calculated)
Year	:	
GLP	:	no data
Test substance	:	other TS: tert-amyl methyl ether (TAME); (CAS #994-05-8)
Method	:	Estimated value, interpolated from measured data (various sources)
Test substance	:	CAS #994-05-8; tert-amyl methyl ether
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data were not reviewed for quality. These data were used for the vapor pressure endpoint in the European Union Risk Assessment for tert-amyl methyl ether (Finnish Environment Institute (2004). 2-Methoxy-Methyl Butane (TAME) Environmental Risk Assessment. Final Draft.).
Flag	:	Critical study for SIDS endpoint

31.07.2006 (15) (16)

Value	:	= 210 hPa at 37.8 °C
Decomposition	:	
Method	:	other (measured)
Year	:	
GLP	:	no data
Test substance	:	other TS: tert-amyl methyl ether (TAME); (CAS #994-05-8)
Method	:	Neste Method 103 using SETVAC apparatus.
Remark	:	Mean of duplicate determinations, SD = 10

Test substance	:	CAS #994-05-8; tert-amyl methyl 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. These data were used for the vapor pressure endpoint in the European Union Risk Assessment for tert-amyl methyl ether(Finnish Environment Institute (2004). 2-Methoxy-Methyl Butane (TAME) Environmental Risk Assessment. Final Draft.).

31.07.2006 (15)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	= 1.55 at 20 °C
pH value	:	
Method	:	OECD Guide-line 117 "Partition Coefficient (n-octanol/water), HPLC Method"
Year	:	1989
GLP	:	yes
Test substance	:	other TS: tert-amyl methyl ether (TAME); (CAS #994-05-8)
Method	:	Mean of six determinations. SD = 0.021 water : octanol ratios of 1:2, 1:1 and 2:1 were used, and the concentration of TAME determined by gas chromatography after through mixing of the two phases. Volatilisation was controlled by sealed vials and gas tight syringes.
Test substance	:	CAS #994-05-8; tert-amyl methyl 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

31.07.2006 (15) (16) (20)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	= 5468 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	:	
GLP	:	no data
Test substance	:	other TS: tert-amyl methyl ether (TAME); (CAS #994-05-8)
Test condition	:	Water Solubility is calculated by the WSKOW, version 1.41, a subroutine of the computer program EPI SuiteTM, version 3.12, which is 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. A log Kow of 1.55 was used with the model.
Test substance	:	CAS #994-05-8; tert-amyl methyl ether
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPI

SuiteTM (2000). This robust summary has a reliability rating of 2 because the data are calculated and not measured.

Flag : Critical study for SIDS endpoint

31.07.2006 (22)

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	:	= .0000000000052179 cm³/(molecule*sec)
Degradation	:	= 50 % after 24.6 hour(s)
Deg. product	:	
Method	:	other (calculated): Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPI SuiteTM version 3.12
Year	:	
GLP	:	
Test substance	:	other TS: tert-amyl methyl ether (TAME); (CAS #994-05-8)
Method	:	Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPI SuiteTM 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	:	Tertiary-amyl methyl ether has the potential to volatilize to air, based on a relatively high vapor pressure, where it is subject to atmospheric oxidation. In air, tert-amyl methyl ether can react with photosensitized oxygen in the form of hydroxyl radicals (OH-). The computer program AOPWIN (atmospheric oxidation program for Microsoft Windows) (EPI SuiteTM, 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. Based on a 12-hour day, a rate constant of 5.22 E-12 cm3/molecule*sec, and an OH- concentration of 1.5 E6 OH-/cm3, tertiary-amyl methyl ether has a calculated half-life in air of 2.05 days or 24.6 hours of daylight.
Test substance	:	CAS #994-05-8; tert-amyl methyl ether
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

04.08.2006 (22)

Deg. product	:	
Method	:	
Year	:	
GLP	:	
Test substance	:	other TS: tert-amyl methyl ether (TAME); (CAS #994-05-8)
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, 1982).
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, tert-amyl methyl ether is not subject to photolytic processes in the aqueous environment.

Test substance : CAS #994-05-8; tert-amyl methyl ether
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
01.08.2006 (13) (25)

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: tert-amyl methyl ether (TAME); (CAS #994-05-8)

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. Tertiary amyl methyl ether is resistant to hydrolysis because it lacks a functional group that is hydrolytically reactive and Harris (1982) identifies ether groups as generally resistant to hydrolysis. Therefore, hydrolysis will not contribute to the removal of tert-amyl methyl ether from the environment.
Test substance : CAS #994-05-8; tert-amyl methyl ether
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
04.08.2006 (12) (14)

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 =	1.55
Water Solubility =	5468 g/m3
Vapor Pressure =	12,000 Pa
Melting Point =	-81.22° C

Result : Using the Mackay Level I calculation, the following distribution is predicted for tert-amyl methyl ether:

%Distribution	Compartment
97.77	Air
2.16	Water
0.07	Soil
<0.01	Sediment
<0.01	Suspended Sediment
<0.01	Biota

Test substance	:	CAS #994-05-8; tert-amyl methyl ether
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

31.07.2006 (18)

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 cannot 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%	Emissions(kg/hr)
Air	26.2	1000
Water	55.1	1000
Soil	18.6	1000
Sediment	0.1	0

Test condition : Physicochemical data used in the calculation:

Parameter	Value w/ Units
Molecular Weight =	102.18
Temperature =	25° C
Log Kow =	1.55
Water Solubility =	5468 g/m3
Vapor Pressure =	12,000 Pa
Melting Point =	-81.22° C

Reaction Half Lives in hours as predicted using EPI SuiteTM:

Air (gaseous)	46.7
Water (no susp. part.)	360
Bulk Soil	720
Bulk Sediment	3240

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 : CAS #994-05-8; tert-amyl methyl ether

Conclusion : The majority of tert-amyl methyl ether (TAME) 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. TAME 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

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3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type	:	aerobic
Inoculum	:	activated sludge, domestic, non-adapted
Contact time	:	28 day(s)
Degradation	:	4 (±) % after 28 day(s)
Result	:	other: not readily biodegradable
Deg. product	:	
Method	:	OECD Guide-line 301 D "Ready Biodegradability: Closed Bottle Test"
Year	:	
GLP	:	yes
Test substance	:	other TS: tert-amyl methyl ether; CAS #994-05-8
Result	:	4.0% degradation was observed after 28 days incubation with an unacclimated inoculum. >60% Degradation of the control substance (sodium benzoate) occurred within 10 days, indicating that the test was valid. % Biodegradation of test substance after days: 2 days = 0 % 7 days = 5 % 14 days = 4 % 21 days = 4 % 28 days = 4 % % Biodegradation of positive control, Benzoic acid, sodium salt: 2 days = 52 % 7 days = 77 %
Test condition	:	OECD Guideline 301 D "Ready Biodegradability: Closed Bottle Test", using 1.99 ± 0.03 mg/l of test substance.
Test substance	:	CAS #994-05-8; tert-amyl methyl ether; purity unknown.
Conclusion	:	tert-Amyl methyl ether is not readily biodegradable.
Reliability	:	(1) valid without restriction

01.08.2006 (7)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

Species	:	other: see remark
Exposure period	:	at 25 °C
Concentration	:	
BCF	:	= 6
Elimination	:	
Method	:	other: calculation
Year	:	
GLP	:	no

Test substance	:	other TS: tert-amyl methyl ether (TAME); (CAS #994-05-8)
Remark	:	A log bioconcentration factor (BCF) of 0.78 is calculated (BCF = 6.0). With respect to a log Kow = 1.92, which was used to calculate the BCF, tert-amyl methyl ether in the aquatic environment is expected to have a low bioaccumulation potential.
Test substance	:	CAS #994-05-8; tert-amyl methyl 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

04.08.2006 (9)

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	flow through
Species	:	Oncorhynchus mykiss (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	= 580
Limit test	:	
Analytical monitoring	:	yes
Method	:	other: U.S. Environmental Protection Agency, Methods for acute toxicity testing with fish, macro-invertebrates and amphibians, TSCA § 797.1400 (EPA-660/3-75-009)
Year	:	1987
GLP	:	yes
Test substance	:	other TS: tert-amyl methyl ether (TAME); CAS #994-05-8

Method : The test guideline followed was TSCA § 797.1400. Twenty organisms (ten per replicate) were exposed in duplicate test aquaria to each of five concentrations of TAME and a dilution water control for 96-hours. During the test, nominal concentrations of 950, 570, 340, 210, and 120 mg A.I./L were maintained by introducing approximately 6.5 aquarium volumes per day of newly prepared test dilution via a modified constant-flow serial diluter apparatus. Each replicate solution was sampled and analyzed for TAME concentration at 0 hours and after 96 hours of exposure. Based on the results of these analyses, the mean measured exposure concentrations were defined as 640, 560, 310, 150, and 78 mg A.I./L. Biological observations and observations of the physical characteristics of the exposure solutions were made and recorded at test initiation and every 24 hours thereafter until the test was terminated. Throughout the exposure period, treatment level solution were observed to be clear and colorless and contained no visible sign of undissolved test material. Test vessels were not covered during the exposure period.

Remark : Statistics: The LC50 was estimated by nonlinear interpolation and 95% confidence intervals were calculated by bionomial probability.

Result : 96-hour LC50 = 580 mg/L based on mean measured values.
72-hour LC50 = 580 mg/L based on mean measured values.
48-hour LC50 = 600 mg/L based on mean measured values.
24-hour LC50 = 600 mg/L based on mean measured values.
96-hour NOEC = 310 mg/L based on mean measured values.

After 72-hours of exposure, 100% mortality was observed among fish exposed to the highest mean measured concentration tested (640 mg/L). At test termination (96 hours), 30% mortality was observed among fish exposed to the 560 mg/L treatment level. In addition, sublethal effects, as defined by darkened pigmentation and equilibrium loss, were observed among all of the surviving fish exposed to this treatment level. No mortality or sublethal effects were observed among fish exposed to the remaining concentrations tested. The NOEC established during this study was 310 mg/L, based on darkened pigmentation and equilibrium loss. There was no control mortality through the test period.

Analytical results:
Nominal treatment levels of 950, 570, 340, 210, and 120 mg A.I./L measured 640, 560, 310, 150, and 78 mg A.I./L, respectively. Both 0- and 96-hour control samples measured <5.3 mg A.I./L. Mean measured concentrations averaged 79% of the nominal concentrations. Coefficients of variation averaged 12% for all mean measured concentrations.

Water quality parameter results:

Temperature ranged between 11 to 12°C through the 96-hour exposure. The pH was 7.1 in all treatment levels and the control at time 0, and pH was 7.2 in all treatment levels and the control at the 24, 48, 72, and 96-hour samplings. Dissolved oxygen ranged from 9.6 to 9.8 mg/L in all treatment levels and the control at time 0, 9.4 to 9.6 mg/L in all treatment levels and the control at time 24, 9.0 to 9.4 mg/L in all treatment levels and the control at time 48, 9.4 to 9.8 mg/L in all treatment levels and the control at time 72, and 8.9 to 9.1 mg/L in all treatment levels and the control at time 96.

Test substance : CAS #994-05-8; tert-amyl methyl ether; 98.8% purity
Reliability : (1) valid without restriction
Guideline study that followed GLP.
Flag : Critical study for SIDS endpoint
01.08.2006 (3)

Type :
Species : other: Fish
Exposure period : 96 hour(s)
Unit : mg/l
LC50 : = 200.6
Method : other: ECOSAR version 0.99h, US EPA
Year :
GLP :
Test substance : other TS: tert-amyl methyl ether; CAS #994-05-8

Method : ECOSAR version 0.99h, U.S. 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 : Calculated 96-hr LC50 for fish = 200.6 mg/L
Test condition : Experimental water solubility, 5468 mg/l @ 20°C (U.S. EPA, 2000), log Kow, 1.55 (Huttunen et al., 1997) and melting point, -82.1°C (U.S. EPA, 2000) were entered into the program.
Class: Neutral organics
Test substance : CAS #994-05-8; tert-amyl methyl ether
Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated and not measured.

31.07.2006 (22)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
EC50	:	= 100
Analytical monitoring	:	yes
Method	:	other: U.S. Environmental Protection Agency, Methods for acute toxicity testing with fish, macro-invertebrates and amphibians, TSCA § 797.1300 (EPA-660/3-75-009).
Year	:	1975
GLP	:	yes
Test substance	:	other TS: tert-amyl methyl ether (TAME); CAS #994-05-8

Method : The test guideline followed was TSCA § 797.1300. Twenty organisms (ten per replicate) were exposed in duplicate test vessels to five concentrations of TAME and a dilution water control for 48 hours. During the test, nominal concentrations of 690, 410, 250, 150, and 89 mg A.I./L were maintained in the exposure vessels by introducing approximately 6.0 test chamber volumes per day of newly prepared test solution via an intermittent-flow proportional diluter apparatus. Each replicate solution was sampled and analyzed for TAME concentration at 0 hours (test initiation) and after 48 hours (test termination) of the exposure period. Based on the results of these analyses, the mean measured exposure concentrations were defined as 120, 83, 55, 28, and 15 mg/l. Biological observations and observations of the physical characteristics of the exposure solutions were made and recorded at test initiation, 6, 24, and 48 hours. Throughout the exposure period, no visible signs of undissolved test material were observed in either the diluter system or in the exposure solutions.

Remark : Statistics: The EC50 was estimated by nonlinear interpolation and 95% confidence intervals were calculated by bionomial probability.

Result : 6-hour LC50 = >120 mg/L based on mean measured values.
24-hour LC50 = >120 mg/L based on mean measured values.
48-hour LC50 = 100 mg/L based on mean measured values.
48-hour NOEC = 83 mg/L based on mean measured values.

After 24-hours of exposure, 15% immobilization was observed among dahpnia exposed to the highest mean measured concentration tested (120 mg/L). At test termination (48 hours), 90% immobilization was observed among daphnia exposed to the 120 mg/L treatment level. In addition, sublethal effects, as defined by lethargy, were observed among all of the surviving daphnia exposed to this treatment level. No immobilization or sublethal effects were observed among daphnia exposed to the remaining concentrations tested. The NOEC established during this study was 83 mg/L, based on lethargy. 5% immobilization occurred in the control at 48 hours. There was no immobilization in the control prior to this sampling point.

Analytical results:
Nominal treatment levels of 690, 410, 250, 150, and 89 mg A.I./L measured 120, 83, 55, 28, and 15 78 mg A.I./L, respectively. Both 0- and 48-hour control samples measured <0.40 mg A.I./L. Mean measured concentrations averaged 19% of the nominal concentrations. Coefficients of variation averaged 11% for all mean measured concentrations. The relatively low recovery obtained for the tested treatment levels (mean=19%) is believed due to the volatile nature of the test material and the size of the test vessels.

Water quality parameter results:
Temperature ranged between 19 to 20°C through the 48-hour exposure. The pH was 8.2 in all treatment levels and the control at time 0, and pH ranged between 8.0 to 8.1 in all treatment levels and the control at the 24 and 48-hour samplings. Dissolved oxygen ranged from 9.1 to 9.2 mg/L in all treatment levels and the control at time 0, 8.7 to 9.1 mg/L in all treatment levels and the control at time 24, and 8.8 to 9.0 mg/L in all treatment levels and the control at time 48. Total hardness as mg/L of CaCO3 ranged from 170 to 190 in the control and treatment levels at test initiation. Total alkalinity ansmg/L CaCO3 ranged from 110 to 120 in the control and treatment levels at test initiation. Specific conductance was 500 umhos/cm in the control and treatment levels at test initiation.

Test substance : CAS #994-05-8; tert-amyl methyl ether; 98.8% purity
Reliability : (1) valid without restriction
Guideline study that followed GLP.
Flag : Critical study for SIDS endpoint
01.08.2006 (1)

Type :
Species : other: Daphnia
Exposure period : 48 hour(s)
Unit : mg/l
EC50 : = 208.4
Method : other: ECOSAR version 0.99h, US EPA
Year :
GLP :
Test substance : other TS: tert-amyl methyl ether; CAS #994-05-8

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 : Calculated 48-hr LC50 for Daphnia = 208.4 mg/L
Test condition : Experimental water solubility, 5468 mg/l @ 20°C (U.S. EPA, 2000), log Kow, 1.55 (Huttunen et al., 1997) and melting point, -82.1°C (U.S. EPA, 2000) were entered into the program.
Class: Neutral organics

Test substance	:	CAS #994-05-8; tert-amyl methyl ether
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated and not measured.

31.07.2006 (22)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	Selenastrum capricornutum (Algae)
Endpoint	:	biomass
Exposure period	:	72 hour(s)
Unit	:	mg/l
NOEC	:	= 77
EbC50	:	= 230
ErC50	:	= 780
Limit test	:	
Analytical monitoring	:	yes
Method	:	OECD Guide-line 201 "Algae, Growth Inhibition Test"
Year	:	
GLP	:	yes
Test substance	:	other TS: tert-amyl methyl ether (TAME); CAS #994-05-8

Method :

The test material was known to be volatile and hence testing was conducted in completely filled, stopperred test vessels in order to minimize possible losses due to volatilization. Following the recommendations in published data (Herman et al. 1990. Aquatic toxicology 18: 87-100.; Mayer et al. 2000. Environmental Toxicology and Chemistry 19: 2551-2556), in order to prevent inhibition of growth due to the restriction of gaseous exchange, additional sodium carbonate was added to the culture medium to provide a source of carbon dioxide for algal growth.

The range-finding test was conducted at nominal test concentrations of 11, 1000, 5000, and 8000 mg/l for 72 hours. Based on the results the following test concentrations were assigned to the definitive test: 100, 200, 400, 800 and 1600 mg/l. At initiation of the test, the culture contained a nominal cell density of 3 E3 cells per ml.

Temperature was maintained at 23 to 25 degrees C throughout the test. The pH values of the control cultures increased from pH 7.5 at 0 hours to pH 8.8 to 8.9 at 72 hours. The test material vessels showed an increase in pH over the 72-hour period following a concentration dependent pattern with the lower test material concentrations exhibiting a greater increase in pH. This effect was considered to be due to there being greater numbers of viable cells in the lower test concentrations and hence greater utilization of carbonate and bicarbonate from photosynthesis/respiration. In all cases, however, the pH shift was less than 1.5 pH unit. No immediate adsorption of the test material to algal cells occurred.

Remark : New genus/species name for the organism tested is Pseudokirchneriella subcapitata.

Result :

72-hour EbC50 = 230 mg/L based on mean measured values.
72-hour ErC50 = 780 mg/L based on mean measured values.
72-hour NOEC = 77 mg/L based on mean measured values.

Results are based on the geometric mean of measured test concentrations. Analysis of the test preparations at 0 hours showed the measured concentrations to range from 83 to 100% of nominal values. After 72 hours there was a slight decline in measured concentrations to 69 to 84% of nominal values. Analysis of samples taken from replicate test vessels that had not been opened during the test period gave measured concentrations of 82 to 96% of nominal values. It was therefore considered that the slight

decline in measured test concentrations observed in the test vessels that had been opened on a daily basis in order to enable samples to be removed for the determination of algal cell density was the result of losses due volatility.

Test substance	:	CAS #994-05-8; tert-amyl methyl ether
Reliability	:	(1) valid without restriction Guideline study that followed GLP.
Flag	:	Critical study for SIDS endpoint

01.08.2006 (11)

Species	:	other algae: Green Alga
Endpoint	:	
Exposure period	:	96 hour(s)
Unit	:	mg/l
EC50	:	= 126.9
ChV	:	= 9.8
Method	:	other: ECOSAR version 0.99h, US EPA
Year	:	
GLP	:	
Test substance	:	other TS: tert-amyl methyl ether (TAME); CAS #994-05-8

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	:	Calculated 96-hr EC50 for a green alga = 126.9 mg/L Calculated 96-hr ChV for a green alga = 9.8 mg/L
Test condition	:	Experimental water solubility, 5468 mg/l @ 20°C (U.S. EPA, 2000), log Kow, 1.55 (Huttunen et al., 1997) and melting point, -82.1°C (U.S. EPA, 2000) were entered into the program. Class: Neutral organics
Test substance	:	CAS #994-05-8; tert-amyl methyl ether
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated and not measured.

31.07.2006 (22)

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	:	ca. 2100 mg/kg bw
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male/female
Number of animals	:	
Vehicle	:	other: None; administered undiluted
Doses	:	
Method	:	other: not specified
Year	:	1995
GLP	:	yes
Test substance	:	other TS: Tertiary Amyl Methyl Ether (TAME) (CAS # 994-05-8)
Remark	:	test type: acute oral toxicity route of administration: oral gavage dose level: variable dose volume: variable
Result	:	LD50 ~ 2.1 g/kg (combined sexes)
Conclusion	:	TAME has a low order of toxicity by the oral route of exposure.
Reliability	:	(2) valid with restrictions

09.10.2006 (8)

5.1.2 ACUTE INHALATION TOXICITY

Type	:	LC50
Value	:	> 5.4 mg/l
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male/female
Number of animals	:	10
Vehicle	:	other: none
Doses	:	5.4 mg/L
Exposure time	:	4 hour(s)
Method	:	other: Not stated
Year	:	1991
GLP	:	yes
Test substance	:	other TS: Tertiary Amyl Methyl Ether (TAME) (CAS # 994-05-8)
Remark	:	Animals were exposed to TAME vapor for 4 hours in a whole body exposure chamber at a concentration of 5.4 mg/L. TAME concentration was measured by infrared absorption. Animals were observed for 14 days post exposure.
Result	:	There were no premature deaths during the course of the study. During the post-mortem evaluation, seven animals showed external hemorrhagic lung foci, with one female having numerous foci (>10). One male had a diffused red area on the lungs. Six animals showed enlarged mandibular lymph nodes. However, the study authors indicated that the observed lung foci were in most cases of a type and number commonly seen in control animals of this strain. LC50 > 5.4 mg/L.
Conclusion	:	TAME has a low order of toxicity by the inhalation route of exposure.
Reliability	:	(1) valid without restriction

09.10.2006 (6)

5.1.3 ACUTE DERMAL TOXICITY

Type	:	LD50
Value	:	> 3160 mg/kg bw
Species	:	rabbit
Strain	:	New Zealand white
Sex	:	male/female
Number of animals	:	6
Vehicle	:	other: none
Doses	:	3160 mg/kg
Method	:	other: Limit test; protocol not stated
Year	:	1985
GLP	:	
Test substance	:	other TS: Tertiary Amyl Methyl Ether (TAME) (CAS # 994-05-8)
Remark	:	TAME was applied neat to the skin of each animal at a dose level of 3160 mg/kg. An occlusive patch covered the test material during the 24 hour exposure period. Animals were observed for 14 days post exposure.
Result	:	There were no premature deaths during the study. However, it was irritating to the skin of the rats. Very slight to severe erythema and slight to very slight edema were observed in all animals. Desquamation was seen in all animals on days 10 and 14; eschar was seen in five animals and atonia in three animals. One animal showed blanching on day 3. At necropsy, desquamation was noted in two animals and another was considered to be slightly emaciated.
Conclusion	:	TAME was of low dermal toxicity in rats. LD50 > 3160 mg/kg.
Reliability	:	(1) valid without restriction

09.10.2006 (10)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

Type	:	other: Skin sensitization
Species	:	other: guinea pig - Dunkin Hartley
Number of animals	:	
Vehicle	:	other: none
Result	:	not sensitizing
Classification	:	not sensitizing
Method	:	other: TSCA TG 798.4100 (Buehler method)
Year	:	1995
GLP	:	yes
Test substance	:	other TS: Tertiary Amyl Methyl Ether (TAME) (CAS: 994-05-8)
Remark	:	Route of administration: Dermal Dose volume: 0.3 ml neat Control group included: Positive and negative controls included Number of animals: Test group--10/sex; Control group--5/sex
Result	:	TAME was non-sensitizing to the skin of guinea pigs

Test condition	:	During the induction phase (days 1, 8 and 15), TAME (approximately 0.3 ml) was applied to the clipped area on the back of the test animals for 6 hours, using an occlusive chamber. Excess material was wiped off at the conclusion of each exposure. The control animals received mineral oil in place of the test chemical under similar conditions. During the challenge phase (day 29), TAME was applied to a clipped area on the back which had not previously been exposed for 6 hours, using an occlusive chamber; a vehicle control (mineral oil) was also used; a further previously untreated group of 5/sex was used as irritation control.
Test substance	:	Tertiary Amyl Methyl Ether (CAS No. 994-05-8) Chemical Name: butane, 2-methoxy-2-methyl- Source/purity not specified.
Conclusion	:	TAME is not a dermal sensitizer
Reliability	:	(1) valid without restriction

01.08.2006 (2)

5.4 REPEATED DOSE TOXICITY

Type	:	Sub-chronic
Species	:	rat
Sex	:	male/female
Strain	:	Sprague-Dawley
Route of admin.	:	other: Inhalation, whole body
Exposure period	:	6 hours/day
Frequency of treatm.	:	5 days/week for 4 weeks
Post exposure period	:	18 hour fasting period
Doses	:	0, 500, 2000 and 4000 ppm
Control group	:	yes
NOAEL	:	= 500 ppm
Method	:	
Year	:	1995
GLP	:	
Test substance	:	other TS: Tertiary Amyl Methyl Ether (TAME) (CAS # 994-05-8)

Remark :

Number of animals: 14/sex/dose group
Sprague-Dawley rats were exposed to 0, 500, 2000 and 4000 ppm TAME for 6 hours per day, 5 days per week for 4 weeks. Animals were observed at least once daily for mortality or obvious signs of toxicity. Body weights were measured at the initiation of the study, weekly during the exposure, and immediately before termination of the animal. All rats were fasted for approximately 18 hours following the final exposure to TAME and anesthetized with sodium pentobarbital. Blood samples were obtained for serum chemistry and hematology parameters.

In addition to daily observation for general toxicity, the study included a functional observational battery (FOB) to evaluate neuromuscular function and sensory perception. The FOB was performed 1 week prior to the first exposure and after 1, 5, or 20 exposures. Four TAME-exposed animals were evaluated approximately 1 hour after the end of exposure and 10 animals were examined the following morning in each exposure group. The FOB consisted of an evaluation of the following parameters: tail pinch, rotorod performance, body temperature, righting reflex, auditory response, hindlimb extension, foot splay, grip strength, home-cage observation, hand-held observation, open-field observation, extensor thrust, catalepsy, visual placing, tactile placing, negative geotaxis, vision, eyeblink, and pupil response.

Necropsies were performed on 10 of the TAME-exposed rats. The following tissues were weighed and fixed in 10% neutral buffered formalin:

brain, adrenal glands, gonads, heart, kidneys, liver, lungs and spleen. Approximately 31 other tissues were also collected and fixed at necropsy. Only those from the high exposure and control groups were processed for histological examination.

For all quantitative parameters, the data were analyzed using both multivariate and univariate two-factor fixed-effects analyses of variance. Quantal data for functional observational battery (FOB) parameters were analyzed using chi-square. A minimum significance level of $P<0.05$ was used in all comparisons.

Result : Three out of 14 males and 4 out of 14 females exposed to 4000 ppm TAME died on test. The deaths were apparently due to severe central nervous system (CNS) depression as there were no gross or histopathology changes to indicate organ-specific tissue injury.

Clinical observations in both the 2000 and 4000 ppm TAME-exposed groups included sedation, coma, ataxia, coldness to touch, ptosis, hyperirritability, hypoactivity and effects on posture. The incidence and severity of effects were greater in the high dose animals. The FOB assessment confirmed the clinical observations. TAME-exposed animals evaluated 1 hour after exposure, especially the 4000 ppm group, displayed reductions in tail pinch response, righting reflex and negative geotaxis, along with reduced body temperature, impaired rotorod performance and increased hindlimb splay. The signs of CNS depression were absent in animals examined 18 hours after the end of exposure. .

Body weight gain was significantly reduced only in male rats exposed to 4000 ppm TAME. Exposure to 2000 and 4000 ppm TAME caused an increase in relative liver weights in males and females. Many relative organ weights were increased for the 4000 ppm males due to the reduced body weights of these animals.

No treatment-related histopathological findings were noted. Clinical chemistry and hematology findings were minimal with TAME. Increased serum cholesterol was found in both male rats (at 2000 and 4000 ppm) and female rats (at 4000 ppm) exposed to TAME. The 4000 ppm males also had reduced serum triglycerides. A single male rat in the 4000 ppm group had an increase in serum alanine aminotransferase (ALT). This animal also displayed multifocal hepatocellular necrosis that can be associated with elevated ALT. The significance of this finding is unclear as this occurred in only one of the seven animals examined. (Three animals had died on test due to CNS depression.)

Conclusion : The NOAEL for subchronic toxicity was 500 ppm in both males and females.

Reliability : (2) valid with restrictions
09.10.2006 (24)

Type	:	Sub-chronic
Species	:	rat
Sex	:	male/female
Strain	:	Sprague-Dawley
Route of admin.	:	other: Oral, gavage
Exposure period	:	
Frequency of treatm.	:	7 days/week for 29 days
Post exposure period	:	
Doses	:	0, 125, 500 and 1000 mg/kg/day
Control group	:	yes
NOAEL	:	= 500 mg/kg
Method	:	other
Year	:	1995
GLP	:	yes
Test substance	:	other TS: Tertiary Amyl Methyl Ether (TAME) (CAS # 994-05-8)

Remark : Number of animals: 5/sex/dose group
Sprague-Dawley rats were exposed to 0, 125, 500 and 1000 mg/kg/day TAME in corn oil by gavage at a dose volume of 2 ml/kg. Vehicle control animals received corn oil only. The dosing regimen was once daily, 7 days a week for a period of 29 days.

Observations were made daily for overt signs of toxicity. Body weights were recorded prior to the first dosing and weekly thereafter during the test period. Food consumption was measured weekly over the course of the study. At study termination, blood samples were collected from all animals (after an overnight fast) for routine hematology and serum chemistry determinations. A complete necropsy was carried out on all animals, and organ weights were obtained for the kidneys, adrenals, liver, testes and ovaries. The following tissues were preserved in 10% neutral buffered formalin: kidneys, adrenals, liver, heart, spleen, ovaries, testes and any tissues appearing abnormal. All tissues preserved from the control and high-dose group, as well as those from animals that died during the study, were processed, sectioned, stained with hematoxylin and eosin and examined microscopically.

Data from the treated groups were compared to those of the control group using the following tests. Comparisons were limited to within-sex analysis. Bartlett's test of homogeneity of variance was used to determine if the groups had equivalent variance at the 1% level. If the variances were not statistically different, the groups were compared using a standard one-way analysis of variance. If significant differences among the means were indicated, Dunnett's test was used to determine which treatment groups differed from controls. Where groups did not have equivalent variance, the non-parametric Kruskall-Wallis test was used to assess differences in group means. If the means were different, Dunn's summed rank test was used to determine which treatment group differed from control.

Result : Four animals (two males, two females) in the high-dose (1000 mg/kg/day) group died during the course of the study. Of these four, two deaths were attributed to dosing accidents. The remaining two deaths were presumed to be test-material related, although a precise cause of death could not be identified. All other animals survived to the scheduled termination.

For the most part, in-life observations were unremarkable. Lung rales and anogenital staining of the fur were observed at a low frequency in the high-dose group. The majority of animals of either sex did not exhibit any unusual symptoms or behaviors.

Overall increases in body weight were noted for all groups of animals. However, mean body weights of high-dose males were significantly lower than those of control males at day 7, day 21 and day 28. Mean body weight gain in high-dose females was also lower than in control females, although the difference was not statistically significant. Food consumption in high-dose males and females was also significantly reduced compared to controls during week 1. During week 2, food consumption was significantly reduced only in high-dose males.

A dose-related increase in adrenal weights (absolute and relative weights) was observed that was statistically significant in the mid- and high-dose males. A similar increase in adrenal weights was not observed in female rats dosed with TAME. Relative kidney weights were also increased in mid- and high-dose male rats compared to control.

Hematology and serum chemistry values were generally similar across groups. Activated partial thromboplastin time was statistically increased in the high-dose male (but not female) group. However, this small increase was not believed to be biologically meaningful. The mean serum glucose

value was also significantly reduced in the high-dose male group. The biological significance of this finding was unknown, however a similar decrease in serum glucose was not observed in high-dose females.

No treatment-related tissue lesions were observed during the histopathological examination. Any changes observed were limited to naturally occurring lesions that were present in approximately equal frequency in all groups, including controls. It was noteworthy that the organ weight increases observed in the kidney and adrenals were not accompanied by any histopathological changes.

Conclusion : The NOAEL for subchronic toxicity was 500 mg/kg/day in both males and females.

Reliability : (1) valid without restriction
09.10.2006 (8)

Type : Sub-chronic
Species : rat
Sex : male/female
Strain : Fischer 344
Route of admin. : other: Inhalation, whole body
Exposure period : 6 hours/day
Frequency of treatm. : 5 days/week for 13 weeks (minimum 65 exposures)
Post exposure period : 4 week recovery period
Doses : 0, 250, 1500 and 3500 ppm
Control group : yes
NOAEL : = 1500 ppm
Method : other: TSCA TG 798.2450; US EPA TG 40 CFR Part 798 Subpart G
Year : 1997
GLP :
Test substance : other TS: Tertiary Amyl Methyl Ether (TAME) (CAS # 994-05-8)

Remark : Fischer 344 rats were exposed to 0, 250, 1500 and 3500 ppm TAME for 6 hours per day, generally 5 days per week for 13 weeks (minimum 65 exposures). Groups of 10/sex at 0 ppm and 3500 ppm were allowed a 4 week recovery period. A satellite group of 10/sex/dose was used for acute neurological testing.

Animals were observed twice daily for mortality or obvious signs of toxicity, and given a detailed examination each week. Body weight and food consumption measurements were performed twice pre-test and weekly during the study. Ophthalmology evaluations were performed pre-exposure, at termination and at the end of the recovery period. Neurobehavioral studies were performed pre-test and on weeks 2,3,5,9 and 14. Hematology and serum chemistry evaluations were performed during weeks 5 or 6, week 14 and following recovery. Cell proliferation was assessed in kidney by examination of incorporation of 5-bromo-2'-deoxyuridine after 1, 4 and 13 weeks exposure to TAME. Nephropathy was evaluated by the presence of hyaline droplets, and specific staining for a2µ-globulin in the proximal convoluted tubules. Animals were subject to a full macroscopic examination at autopsy, and selected organs weighed, sampled and preserved for all animals. Selected tissues from the control and high dose rats were processed, stained and examined by light microscopy.
Number of animals: 51/sex for the control and high dose groups; 41/sex for the low and mid dose groups

Result : A number of effects were observed at the highest dose used, 3500 ppm. These included two deaths, post-exposure clinical signs, acute neurological effects, decreased body weight and body weight gain, increased platelet counts, increases in total protein, albumin and globulin, and a number of effects on organ weights. Many of these resolved after the 4 week recovery period. There were effects on the body weight and brain weight of males after this time. The effects on the kidneys of the male rats were

consistent with the male rat specific a2µ-globulin syndrome and were not considered to be relevant to risk assessment in humans.

Exposure of rats at 1500 ppm resulted in effects including post exposure clinical signs, acute neurological effects (males only), increased platelet count in males, increases in total protein, albumin and globulin and effects on liver and kidney (only in females) weight. An increase in liver weights of male rats exposed to 250 ppm was also observed. Many of these resolved after the 4 week recovery period.

No test material related changes in motor activity were observed at any doses. Functional observational battery (FOB) tests were performed on the satellite group 1, 6 and 24 hours after acute exposure. Central nervous system (CNS) depression, indicated by postural changes, drooping or half-closed eyelids, slight stupor or lack of reflex responses, and lack of neuromuscular coordination, indicated by ataxia, impaired locomotion, poor righting reflex, reduced grip strength and increased landing foot splay, were seen in most 3500 ppm animals and a few 1500 ppm males after 1 hour. After 6 hours, one 3500 ppm male was in a low arousal state and a slight decrease in hindlimb grip strength in the 3500 ppm females was observed. After 24 hours, the FOB test results for all groups were comparable to controls.

Following repeated exposures for a second satellite group of 10/sex/dose, an increase in forelimb grip strength was recorded in the 3500 ppm males and 1500 and 3500 ppm females. No other effects on measures of neuromuscular function or CNS depression were observed.

Microscopic examination of the brain, spinal cord (cervical, thoracic, lumbar) and sciatic, sural and tibial nerves showed no evidence of any treatment-related effects.

The increased severity of hypertrophy/hyperplasia of the goblet cells in the respiratory mucosa and in the epithelium lining the nasopharynx was observed in the 3500 ppm group. This effect was considered to be a localized adaptive response to a minimal irritant effects rather than an adverse toxicological response to the test material. Similar responses have been seen in rats exposed to mild irritants such as cigarette smoke, formaldehyde, and ammonia.

Conclusion : The NOAEL for subchronic toxicity was 1500 ppm in both males and females.

Reliability : (1) valid without restriction
09.10.2006 (4)

Type	:	Sub-chronic
Species	:	mouse
Sex	:	male/female
Strain	:	CD-1
Route of admin.	:	inhalation
Exposure period	:	6 hours/day
Frequency of treatm.	:	5 days/week for 13 weeks
Post exposure period	:	4 week recovery period
Doses	:	0, 250, 1500 and 3500 ppm; due to high incidence of mortality at 3500 ppm early in the study, the high dose was eventually set at 2500 ppm (i.e., new high dose and control groups were established)
Control group	:	yes
NOAEL	:	= 1500 ppm
Method	:	other: TSCA TG 798.2450; US EPA TG 40 CFR Part 798 Subpart G
Year	:	1997
GLP	:	yes
Test substance	:	other TS: Tertiary Amyl Methyl Ether (TAME) (CAS # 994-05-8)

Remark	:	CD-1 mice were exposed to 0, 250, 1500 and 3500 ppm TAME initially; a new high dose group of mice at 2500 ppm and corresponding control group were established due to high mortality at 3500 ppm. Exposures were for 6 hours per day, generally 5 days per week for 13 weeks (minimum 65 exposures); groups of 10/sex at 0 ppm and the highest dose, 2500 ppm were allowed a 4 week recovery period. Animals were observed twice daily for mortality or obvious signs of toxicity, and given a detailed examination each week. Body weight and food consumption measurements were performed twice pre-test and weekly during the study. Ophthalmology evaluations were performed pre-exposure, at termination and at the end of the recovery period. Hematology and serum chemistry evaluations were performed during weeks 5 or 6, week 14 and following recovery. Cell proliferation was assessed in liver by examination of incorporation of 5-bromo-2'-deoxyuridine after 1, 4 and 13 weeks exposure to TAME. Animals were subject to a full macroscopic examination at autopsy, and selected organs weighed, sampled and preserved for all animals. Selected tissues from the control and high dose rats were processed, stained and examined by light microscopy. Number of animals: 46/sex for the control and high dose groups (two groups each); 36/sex for the low and mid dose groups
Result	:	At 3500 ppm, 13 of 46 males and 10 of 46 females died after the first exposure and 26 of 46 males and 14 of 46 females died within three exposures to TAME. A trial was conducted with groups of 15 mice/sex exposed at 3000 ppm; 8 males and 4 females died within eight exposures. Accordingly the high dose was set at 2500 ppm. A number of effects were observed at the highest dose used in the main study, 2500 ppm. These included 27 deaths among 92 mice, post-exposure clinical signs, effects on a number of clinical chemistry parameters, and increased liver weights. Many of these resolved after the 4 week recovery period. Liver cell proliferation studies showed increases in the labelling index of hepatocytes and centrilobular hepatocellular hypertrophy was observed in both sexes. Exposure of mice at 1500 ppm resulted in effects including post exposure clinical signs, increased globulin in males at week 6 and effects on liver weights in males. Similar findings were made in the liver cell proliferation studies and microscopic examination to those for the 2500 ppm animals. These liver effects were also observed for female mice exposed to 250 ppm. Centrilobular hepatocellular hypertrophy is frequently seen in the liver following exposure to agents that cause hepatic enzyme induction. Therefore, this effect is considered an adaptive response to increased metabolic load.
Conclusion	:	The NOAEL for subchronic toxicity was 1500 ppm in both males and females.
Reliability	:	(1) valid without restriction

09.10.2006 (4)

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Bacterial reverse mutation assay
System of testing	:	Salmonella typhimurium
Test concentration	:	Doses ranging from 100 to 10,000 ug per plate
Cycotoxic concentr.	:	>10,000 ug/plate
Metabolic activation	:	with and without
Result	:	negative

Method	:	other: EPA OTS 798.5265, Similar to OECD Guideline 471
Year	:	1995
GLP	:	yes
Test substance	:	other TS: Tertiary Amyl Methyl Ether (TAME) (CAS # 994-05-8)
Remark	:	Strains tested: Salmonella typhimurium tester strains TA98, TA100, TA1535, TA1537, TA1538 Test substance doses/concentration levels: The concentration of TAME ranged from 100 to 10,000 ug per plate Metabolic activation: With and without (S9 fraction mix of livers of Aroclor 1254 pretreated rats) Vehicle: Dimethyl sulfoxide (DMSO) Positive Controls: 2-aminoanthracene (5 ug/plate); 9-aminoacridine (100 ug/plate); N-methyl-N-nitro-N-nitrosoguanidine (MNNG) (10 ug/plate) and 2-nitrofluorene (5 ug/plate). Statistical analysis: Mean revertant colony count (means of triplicate plates) were determined for each dose point. Cytotoxicity study: A toxicity screening test conducted prior to the full assay indicated a lack of toxicity at concentrations as high as 10,000 ug per plate.
Result	:	TAME did not induce reverse gene mutation in any strain. The test substance was not genotoxic in this assay with or without metabolic activation. A satisfactory response was obtained with the positive control substances (2-aminoanthracene, 9-aminoacridine, MNNG, 2-nitrofluorene).
Conclusion	:	Under the conditions of this study, the test material was not mutagenic.
Reliability	:	(1) valid without restriction

09.10.2006 (8)

Type	:	other: Mammalian Chromosomal Aberration Test
System of testing	:	Chinese hamster ovary cells (CHO)
Test concentration	:	313, 625, 1250, 2500 and 5000 ug/ml
Cycotoxic concentr.	:	5000 ug/ml
Metabolic activation	:	with and without
Result	:	positive
Method	:	other: OECD Guideline 473
Year	:	1997
GLP	:	no data
Test substance	:	other TS: Tertiary Amyl Methyl Ether (TAME) (CAS # 994-05-8)
Remark	:	Metabolic activation: With and without rat liver S9 from animals pretreated with Arochlor 1254 Test type: Chromosome damage CHO cells were treated with 313, 625, 1250 and 5000 ug/ml TAME in the presence and absence of rat liver S9. Cells were treated with TAME for 12 hours in the absence of S9 (-S9) and for 4 hours with a 16 hour recovery period in the presence of S9. Mitomycin C was used as the positive control for experiments conducted in the absence of S9 whereas cyclophosphamide was used as the positive control for experiments conducted in the presence of S9. Ethanol was the negative control in all experiments. Colcemid (0.1 ug/ml) was added 2 hours before harvest to arrest cells in metaphase. TAME was soluble in the treatment medium at all doses tested.

In the absence of S9, a statistically significant increase in aberrant cells was observed at 2500 and 5000 ug/ml, and a dose response was observed. In the presence of S9, a statistically significant increase in aberrant cells was observed at all concentrations and a dose response was observed.

The positive controls caused large, statistically significant increases in the proportion of aberrant cells in all cases, indicating that the test system responded appropriately.

Conclusion : TAME was clastogenic under the conditions of this test.
Reliability : (1) valid without restriction
09.10.2006 (5)

5.6 GENETIC TOXICITY 'IN VIVO'

Type : other: Mammalian Erythrocyte Micronucleus Test
Species : mouse
Sex : male/female
Strain : CD-1
Route of admin. : other: Intraperitoneal injection
Exposure period : Bone marrow (femur) sampled at 24hr, 48hr, 72hr after administration (24hr only for the positive control substance)
Doses : 0.15, 0.375, 0.75 g/kg
Result : negative
Method : other: EPA OTS 798.5395, Similar to OECD Guideline 474
Year : 1995
GLP : yes
Test substance : other TS: Tertiary Amyl Methyl Ether (TAME) (CAS # 994-05-8)

Remark : Tertiary amyl methyl ether was diluted in corn oil and administered as a single intraperitoneal (i.p.) injection at doses of 0.75, 0.375 and 0.15 g/kg body weight. Cyclophosphamide was dissolved in water and used as the positive control at a dose of 40 mg/kg i.p.

Animals from the appropriate groups were euthanized by CO2 at ca. 24, 48 and 72 hours after administration of test article. Animals dosed with cyclophosphamide were taken at 24 hours only. Each group consisted of 10 animals (five per sex) per time point. At death, both femurs from each animal were removed and bone marrow was recovered and suspended in fetal bovine serum. Following centrifugation to pellet the tissue, the supernatant was drawn off, the pellet resuspended and the suspension spread on slides and dried (two slides were prepared per animal). Prior to microscopic evaluation, the slides were stained using acridine orange.

One thousand polychromatic erythrocytes from each animal were examined for micronuclei formation. Criteria for scoring micronuclei were those of Schmid. In addition, the ratio of polychromatic erythrocytes (PCEs) to normochromatic erythrocytes (NCEs) was determined by counting 1000 erythrocytes (PCEs and NCEs). The data were evaluated statistically using ANOVA.

Result : All mice survived to scheduled termination. No increase in micronucleus frequency was observed at any dose level of TAME or at any of the bone marrow collection times. The positive control (cyclophosphamide) produced statistically significant increases in micronucleus frequencies in both males and females. Overt marow toxicity, as measured by a statistically significant decrease in the percentage of polychromatic erythrocytes, was not observed in any of the groups dosed with TAME. The percentages of polychromatic erythrocytes observed were within the normal range. Thus, these data indicated that TAME did not cause

clastogenic effects in mouse bone marrow.

Conclusion : TAME did not produce clastogenic effects in mouse bone marrow.
Reliability : (1) valid without restriction
09.10.2006 (8)

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

Type : other: Two-generation Reproductive Toxicity Test
Species : rat
Sex : male/female
Strain : Sprague-Dawley
Route of admin. : other: Whole body inhalation
Exposure period : Males: premating, mating, postmating (30 days); Females: premating, mating through gestational day 19, lactation (postnatal day 5 through 28)
Frequency of treatm. : 6 hr/day, 5-7 days/week
Premating exposure period
Male : 5 days/week for 10 weeks
Female : 5 days/week for 10 weeks
Duration of test : 43 weeks
No. of generation studies : 2
Doses : 250, 1500 and 3000 ppm
Control group : other: Yes - air-exposed
Method : other: OPPTS - 1996 draft guidelines
Year : 2003
GLP : yes
Test substance : other TS: Tertiary Amyl Methyl Ether (CAS # 994-05-8)

Remark : The study began with 30 males and 30 females per group to yield at least 20 pregnant females per group at or near term. Exposure began for all F0 animals when they were ca. 7 weeks old. Animals were assigned to groups by means of randomization stratified by body weight, such that the body weights by gender of all groups were homogeneous by statistical analysis at study initiation.

The study was conducted with three treatment groups and an air (vehicle control) group, each comprising 30 rats/gender. The target exposure concentrations were 250, 1500 and 3000 ppm. The F0 animals (parents of the F1 generation) and selected F1 offspring (parents of F2 generation) were exposed to TAME vapor for 6 hr/day, 5 days/week, during the premating exposure periods (for at least 10 weeks) and the postmating holding period (males, for ca. 30 days). During mating (both genders), gestation (dams) and lactation (dams) of F1 and F2 litters, exposures were 6 hr/day, 7 days/week. Pregnant dams were not exposed beginning on gestational day (gd) 20. Dams with litters were not exposed on postnatal day (pnd) 0 (day of parturition) through to pnd 4. Exposures to the dams resumed on pnd 5. Retained postwean F2 offspring were not exposed to TAME vapor.

Observations for mortality were made twice daily and clinical examinations were conducted and recorded daily, prior to and after each exposure period, through the course of the study. The body weights of male rats were recorded initially and weekly through mating. The body weights of female rats were recorded in the same manner until confirmation of mating. Females were weighed and the feed consumption was recorded on gd 0, 7, 14 and 20 and on pnd 0, 4, 7, 14, 21 and 28. For the last three weeks of

the premating exposure period, vaginal smears were taken for all F0 and F1 females. The slides from the premating period were evaluated for estrous cyclicity and normality. Vaginal smears were taken daily during the 14-day mating period or until mating was confirmed. The observation of vaginal sperm or copulation plug was considered evidence of successful mating.

All pups (F1 and F2 litters) were counted, weighed, sexed and examined as soon as possible after birth to determine the number of viable and stillborn members of each litter. Thereafter, all live pups were counted, their gender determined, weighed individually and examined grossly, and litters were evaluated for survival on pnd 4, 7, 14 and 21 and at weaning (pnd 28).

Statistical method:
The unit of comparison was the male, the female, the pregnant female or litter, as appropriate. Quantitative continuous data (e.g. parental and pup body weights, organ weights, F2 anogenital distance, feed consumption, food efficiency, etc.) were compared among the three treatment groups and the one vehicle control group by the use of Bartlett's test for homogeneitiy of variances. If Bartlett's test indicated a lack of homogeneity of variances (i.e. P<0.001), then non-parametric statistical tests were employed for the continuous variables. Non-parametric tests, used for continuous data that did not have homogeneous variances, included the Kruskal-Wallis test to determine whether significant differences were present among the groups, followed by the Mann-Whitney U test for pairwise comparisons to the vehicle control group if the Kruskal-Wallis test was significant. Jonckheere's test for k independent samples was used to identify significant dose-response trends for non-parametric continous data. If Bartlett's test indicated homogeneous variances (i.e. P>0.001), then parametric statistical tests were employed for the continuous variables. A general linear model (GLM) procedures for the analysis of variance (ANOVA) were used to determine the significance of the dose-response relationship and to determine whether significant dosage effects had occurred for selected measures. For all statistical tests, the significance limit of 0.05 was used as the criterion for significance. A test for statistical outliers was performed on parental body weights and feed consumption (in g/day). If examination of pertinent study data did not provide a plausible and biologically sound reason for inclusion of the data flagged as "outlier," the data were excluded from summarization and analysis and were designated as outliers. If feed consumption data (in g/ day) were negative for a given animal and period, they were designated "unrealistic" and excluded from summarization and analysis. If feed consumption data for a given observational interval (e.g. study days 0-7, 7-14, 14-28, 28-35, etc.) during the premating exposure period were designated outliers or unrealistic, then summarized data encompassing this period (e.g. study days 0-70 for the premating exposure period) also did not include this value.

Result : Adult systemic toxicity was present for F0 and F1 parental animals at 1500 and 3000 ppm. At 3000 ppm, there were consistent and persistent reductions in body weights, weight gains and feed consumption (in g/day) in both genders and both generations. Feed consumption (in g/kg/day) and food efficiency were variable. Clinical observations at 3000 ppm were limited to ataxia (during and immediately after exposures) in most to all animals in both genders and both generations. Body weights during gestation in F1 dams and during lactation in F0 and F1 dams were reduced at 3000 ppm. At 1500 ppm, there were no effects on body weights, feed consumption or food efficiency, but ataxia was present in F0 males and females and lactational weight change was reduced in F1 dams.

At necropsy, parental absolute and relative liver weights were increased in both genders and generations at 3000 ppm (in F0 males, absolute and

relative kidney weights also were increased at 250 and 1500 ppm). Relative (but not absolute) spleen weights also were increased at 3000 ppm. Brain weights, absolute or relative, were not consistently affected. There were no treatment-related gross or histopathological findings for any of these organs.

Reproductive toxicity:
Adult reproductive toxicity was minimally present at 3000 ppm in males, expressed as reduced body weights throughout premating and mating and increased relative (but not absolute) testes weights in F0 and F1 males, most likely due to reduced terminal body weights at this concentration, reduced absolute prostate weight in F1 (but not F0) males, reduced epididymal sperm concentration in F1 (but not F0) males and significantly increased percentage of abnormal sperm in F0 (but not in F1) males. At 1500 ppm, the percentage of abnormal sperm was increased relative to the concurrent control value in F0 males, but this value was well within the historical control range for this parameter. There were no effects of treatment on mating or survival indices, absolute testes weight, absolute or relative weights of the epididymides or seminal vesicles with coagulating gland, relative prostate weight, percentage of motile or progressively motile sperm, testicular homogenization-resistant spermatid head counts, daily sperm production or efficiency of daily sperm production. There were also no treatment-related gross or histopathological findings in the reproductive organs in F0 or F1 males.

In F0 and F1 females there were no effects of treatment on vaginal cyclicity, estrous cycle length, mating, fertility, pregnancy, gestational indices or gestational length. Cycle length was reduced at 1500 ppm but not at 3000 ppm in F1 females, and not in F0 females at any concentration. This is most likely due to biological variation. Gestational length was significantly longer than the concurrent control values at 1500 ppm, with no effects at 3000 ppm in F1 females and no effects in F0 females at any concentration. The values were all well within the historical control range for this parameter. There were also no effects on number of implantation sites per litter, on number of total, live or dead pups per litter on pnd 0 or on the percentage of postimplantation loss per litter (prenatal mortality index). There were also no effects on absolute or relative ovary or uterine weight and no treatment-related gross or histopathological findings in these organs.

Offspring toxicity:
Offspring toxicity was present at 1500 and 3000 ppm. Survival indices were unaffected for F1 offspring throughout lactation (pnd 4, 7, 14, 21 and 28) and were unaffected for F2 offspring for pnd 7, 14 and 28. The F2 survival indices were significantly reduced at 3000 ppm for pnd 4 and 21. The F1 pup body weights per litter were significantly reduced during lactation at 1500 and 3000 ppm on pnd 4, 7, 14, 21 and 28 (but not on pnd 0) and at 250 ppm on pnd 14, 21 and 28 (the last only for males). The F2 pup body weights per litter were significantly reduced during lactation at 3000 ppm for pnd 0, 4, 7, 14, 21 and 28 and at 1500 ppm for pnd 14 and 21. There were no effects on the F2 pups at 250 ppm. Delays (not correlated with body weight differences) in the age of preputial separation in males (F1 at 1500 and 3000 ppm, and F2 at 3000 ppm) and vaginal patency in females (F1 at 3000 ppm, and F2 at 250 and 3000 ppm) were observed in both generations. Overall the effects seemed more severe on the F1 generation. Shorter anogenital distances at birth were observed in both sexes of the F2 generation. These appeared to be related to lower birth weights. The pattern exhibited by these results was considered more likely to be due to overall toxicity, rather than endocrine disruption, which would be expected to have more severe effects on one sex than the other.

Conclusion : Exposure to TAME vapor for 6 hr/day, 5-7 days/week for two generations, one litter per generation, at 0, 250, 1500 and 3000 ppm resulted in

systemic effects at 1500 and 3000 ppm, minimum adult reproductive toxicity at 3000 ppm and offspring toxicity at 1500 and 3000 ppm. The NOAEL for adult reproductive toxicity was 1500 ppm for males and 3000 ppm for females. The NOAEL for offspring toxicity was 250 ppm in rats under the conditions of this study.

Reliability : (1) valid without restriction
09.10.2006 (21)

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 6-19 (14 consecutive days)
Duration of test	:	14 days
Doses	:	0, 250, 1500, or 3500 ppm
Control group	:	other: yes (air-exposed)
NOAEL maternal tox.	:	= 250 ppm
other: NOAEL Pupl	:	= 1500 ppm
Result	:	Maternal NOAEL: 250 ppm; Pup NOAEL: 1500 ppm
Method	:	other: EPA OPPTS - 1996 draft guidelines
Year	:	2003
GLP	:	yes
Test substance	:	other TS: Tertiary Amyl Methyl Ether (TAME) (CAS # 994-05-8)

Remark : In this study, 25 evidence-of-mating-positive females per group were exposed to TAME for 6 hr/day on 14 consecutive days (gd 6-19). Clinical observations were taken daily, except during the exposure period. During this period they were made at least twice daily, immediately before and after each daily TAME exposure. Maternal body weights were recorded in the morning on gd 0, 6, 9, 12, 15, 18 and 20. Feed consumption was measured for the intervals gd 0-6, 6-9, 9-12, 12-15, 15-18, and 18-20. At scheduled termination on gd 20, the dams were evaluated for body, liver and gravid uterine weights. Ovarian corpora lutea were counted and the status of uterine implantation sites (i.e. resorptions, dead fetuses, live fetuses) was recorded. All fetuses were dissected from the uterus, counted and weighed; their gender was determined and the fetuses were examined for external abnormalities. Approximately half of the fetuses in each litter were examined for visceral malformations and variations by a fresh tissue dissection method. The heads of the fetuses were removed and fixed in Bouin's solution; serial free-hand sections of the heads were examined for soft--tissue craniofacial malformations and variations. All fetuses in each litter were eviscerated, fixed in alcohol and stained with alizarin red S/alcian blue. Intact fetuses (approximately half per litter; the one not examined viscerally or decapitated) were examined for skeletal malformations and variations.

Statistical method:
Quantitative continuous data (e.g. maternal body weights, fetal body weights, maternal feed consumptions, etc.) were compared among the three treatment groups against the air inhalation control group by Bartlett's test for homogeneity of variances. If Bartlett's test indicated lack of homogeneity of variances (i.e. $P<0.001$), then non-parametric statistical tests were employed for the continuous variables. If Bartlett's test indicated homogeneous variances (i.e. $P>0.001$), then parametric statistical tests were used. Parametric statistical procedures that were applied to selected measures from this developmental toxicity study were as follows. Appropriate general linear model (GLM) procedures were used for the

analysis of variance (ANOVA). Prior to GLM analysis, an arcsine square root transformation was performed on all litter-derived percentage data to allow the use of parametric methods. For these litter-derived percentage data, the ANOVA was weighted according to litter size. The GLM analysis was used to determine the significance of the concentration-response relationship (test for linear trend) and to determine whether significant concentration-related effects had occurred for selected measures (ANOVA). When a significant (P<0.05) main effect for concentration occurred, Dunnett's multiple comparison test was used to compare each TAME-exposed group to the control group for that measure. A one-tailed Test (i.e. Dunnett's test) was used for all pairwise differences from the air-only control group, except that a two-tailed test was used for maternal body and organ weight parameters, maternal feed consumption, fetal body weight and percent of males per litter.
Non-parametric tests were used on continuous data without homogeneous variances and included the Kruskal-Wallis test to determine if significant differences were present among the groups, followed by the Mann-Whitney U test for pairwise differences from the designated control group if the Kruskal-Wallis test was significant. Jonckheere's test for k independent samples was applied to identify significant dose-response trends for non-parametric continuous data. Nominal scale measures were analyzed by the chi-square test for independence for differences among treatment groups and by the Cochran-Armitage test for a linear trend on proportions. When the chi-square test revealed significant (P<0.05) differences among groups, a two-tailed Fisher's exact probability test with appropriate adjustment for multiple comparisons was used for pairwise differences between each TAME-exposed group and the control group. A test for statistical outliers was performed on maternal body weights and feed consumption (in g/day). If examination of pertinent study data did not provide a plausible and biologically sound reason for inclusion of the data flagged as "outlier," the data were excluded from summarization and analysis and were designated as outliers. If feed consumption data (in g/day) were negative for a given dam and period, they were designated unrealistic and excluded from summarization and analysis. If feed consumption data for a given observational interval (e.g. gd 6-9, 9-12, 12-15 or 15-17) were designated outliers or unrealistic, then summarized data encompassing this period (e.g. treatment period) also did not include this value.

Result : Maternal toxicity observations:

Prior to the start of exposures, maternal body weights were equivalent across all groups. Maternal body weight was significantly reduced only at 3500 ppm for gd 12, 15, 18 and 20 (in-life and at termination). Maternal weight change was significantly reduced at 1500 and 3500 ppm for gd 6-9 and at 3500 ppm for gd 6-20 (exposure period). Maternal weight change was significantly reduced at 1500 and 3500 ppm for gd 0-20 (entire gestation period), as was gestational weight change corrected for weight of the gravid uterus. There were no effects on maternal weight change at 250 ppm. Gravid uterine weight exhibited a significant exposure-concentration related downward linear trend (P<0.05) but no statistically significant pairwise comparison differences in any group compared with the concurrent control group. Maternal absolute liver weights were equivalent across all groups. At scheduled necropsy, maternal liver weight relative to body weight was significantly increased at 3500 ppm.

Maternal feed consumption (in g/day) was significantly reduced at 3500 ppm for gd 6-9, 9-12, 12-15, 15-18, 18-20, 6-20 (exposure period) and 0-20 (gestation period). At 1500 ppm, feed consumption was significantly reduced only for gd 9-12. When the data were expressed as g/kg/day, maternal feed consumption at 3500 ppm was reduced for gd 6-9, 9-12 and 6-20. At 1500 ppm, feed consumption (as g/kg/day) was significantly reduced only for gd 6-9. There were no effects of treatment on maternal

feed consumption at 250 ppm.

Clinical observations related to TAME exposure at 3500 ppm included ataxia (after exposure on gd 6-11), dazed appearance (gd 6-12), lethargy (gd 6-13 and 16-19), eyes squinted (gd 6-8 and 10), eyes closed (gd 8 and 11), pica (gd 6-14 and 16), slow respiration (gd 6, 8 and 11), piloerection (gd 6, 7, 9, 15, 16, 17 and 19), rough coat (gd 7, 9 and 10), facial tremors (gd 8 and 11), gasping (gd 8) and clinical weight loss (>5.0 g within a weighing period) on gd 9. At 1500 ppm, dams exhibited lethargy (one each on gd 6 and 7) and piloerection (one on gd 15). At 250 ppm, one dam exhibited pica on gd 6 and two dams exhibited piloerection on gd 19. There was a clear indication of maternal accommodation to the highest TAME exposure concentration, as evidenced by diminution in incidence and intensity of clinical signs such as ataxia, lethargy and slow respiration over time. At scheduled necropsy, no gross anomalies were found in dams.

Embryo/fetal toxicity

There were no significant effects of treatment on gestational parameters, including number of ovarian corpora lutea, total number of uterine implantation sites, pre- or post-implantation loss, number of live fetuses per litter and gender ratio (% male fetuses) per litter. Fetal body weight per litter, when calculated as all fetuses,or males or females separately, was significantly reduced at 3500 ppm.

There were no treatment-related changes in the incidence of individual or pooled external, visceral, skeletal or total malformation or variations by litter or by fetus per litter. One fetus in one litter at 250 ppm exhibited all the external malformations observed in the TAME-exposed groups of this study: unilateral right anophthalmia, ocular orbits close together, agenesis of the nostril and micrognathia. Fetal visceral malformations were almost exclusively limited to hydronephrosis and hydroureter, distributed across 0. 250 and 1500 ppm, and one fetus in one litter at 0 ppm with interventricular septal defect. For fetal skeletal malformations, one fetus at 0 ppm exhibited fused sternebrae, one fetus at 1500 ppm exhibited scrambled sternebrae and agenesis of a rib and one fetus at 3500 ppm exhibited bipartite cartilage and bipartite ossification center in the thoracic centrum. Fetal external variations were distributed across all groups and were limited to hematomas at various locations. Fetal visceral variations were distributed across all groups with no TAME exposure-related pattern; they included predominantly enlarged laterl ventricles of the cerebrum and distended ureters, both common findings in term fetuses. Fetal skeletal variations included misaligned sternebrae and changes in cartilage and bone in the thoracic centra, predominantly extra rib (full or rudimentary) on lumbar vertebra no. 1 across all groups examined. These variations are common fetal findings.

Conclusion : There was no evidence of treatment-related teratogenicity at any of the three exposure concentrations and no other developmental effects. Almost all the fetal malformation and variation findings were those commonly observed in historical control Sprague-Dawley rat fetuses and in published control databases. Therefore, the NOAEL was 250 ppm for maternal toxicity and 1500 ppm for developmental toxicity in rats under the conditions of this study.

Reliability : (1) valid without restriction
09.10.2006 (23)

Species : mouse
Sex : female
Strain : CD-1
Route of admin. : inhalation
Exposure period : 6 hr/day
Frequency of treatm. : Gestation Days 6-16 (11 consecutive days)

Duration of test	:	11 days
Doses	:	0, 250, 1500, or 3500 ppm
Control group	:	other: yes (air-exposed)
NOAEL maternal tox.	:	= 250 ppm
other: NOAEL Pup	:	= 250 - ppm
Result	:	Maternal NOAEL: 250 ppm; Pup NOAEL: 250 ppm
Method	:	other: EPA OPPTS - 1996 draft guidelines
Year	:	2003
GLP	:	yes
Test substance	:	other TS: Tertiary Amyl Methyl Ether (TAME) (CAS # 994-05-8)

Remark :

In this study, 25 evidence-of-mating-positive females per group were exposed to TAME for 6 hrs per day on 11 consecutive days (gd 6-16). Clinical observations were taken daily, except during the exposure period. During this period they were made at least twice daily, immediately before and after each daily TAME exposure. Maternal body weights were recorded in the morning on gd 0, 6, 9, 12, 15 and 17. Feed consumption was measured for the intervals gd 0-6, 6-9, 9-12, 12-15, and 15-17. At scheduled termination on gd 17, the dams were evaluated for body, liver and gravid uterine weights. Ovarian corpora lutea were counted and the status of uterine implantation sites (i.e. resorptions, dead fetuses, live fetuses) was recorded. All fetuses were dissected from the uterus, counted and weighed; their gender was determined and the fetuses were examined for external abnormalities. Approximately half of the fetuses in each litter were examined for visceral malformations and variations by a fresh tissue dissection method. The heads of the fetuses were removed and fixed in Bouin's solution; serial free-hand sections of the heads were examined for soft--tissue craniofacial malformations and variations. All fetuses in each litter were eviscerated, fixed in alcohol and stained with alizarin red S/alcian blue. Intact fetuses (approximately half per litter; the one not examined viscerally or decapitated) were examined for skeletal malformations and variations.

Statistical method:
Quantitative continuous data (e.g. maternal body weights, fetal body weights, maternal feed consumptions, etc.) were compared among the three treatment groups against the air inhalation control group by Bartlett's test for homogeneity of variances. If Bartlett's test indicated lack of homogeneity of variances (i.e. P<0.001), then non-parametric statistical tests were employed for the continuous variables. If Bartlett's test indicated homogeneous variances (i.e. P>9.001), then parametric statistical tests were used. Parametric statistical procedures that were applied to selected measures from this developmental toxicity study were as follows. Appropriate general linear model (GLM) procedures were used for the analysis of variance (ANOVA). Prior to GLM analysis, an arcsine square root transformation was performed on all liter-derived percentage data to allow the use of parametric methods. For these litter-derived percentage data, the ANOVA was weighted according to litter size. The GLM analysis was used to determine the significance of the concentration-response relationship (test for linear trend) and to determine whether significant concentration-related effects had occurred for selected measures (ANOVA). When a significant (P<0.05) main effect for concentration occurred, Dunnett's multiple comparison test was used to compare each TAME-exposed group to the control group for that measure. A one-tailed Test (i.e. Dunnett's test) was used for all pairwise differences from the air-only control group, except that a two-tailed test was used for maternal body and organ weight parameters, maternal feed consumption, fetal body weight and percent of males per litter.
Non-parametric tests were used on continuous data without homogeneous variances and included the Kruskal-Wallis test to determine if significant differences were present among the groups, followed by the Mann-Whitney U test for pairwise differences from the designated control group if the

Kruskal-Wallis test was significant. Jonckheere's test for k independent samples was applied to identify significant dose-response trends for non-parametric continuous data. Nominal scale measures were analyzed by the chi-square test for independence for differences among treatment groups and by the Cochran-Armitage test for a linear trend on proportions. When the chi-square test revealed significant ($P<0.05$) differences among groups, a two-tailed Fisher's exact probability test with appropriate adjustment for multiple comparisons was used for pairwise differences between each TAME-exposed group and the control group. A test for statistical outliers was performed on maternal body weights and feed consumption (in g/day). If examination of pertinent study data did not provide a plausible and biologically sound reason for inclusion of the data flagged as "outlier," the data were excluded from summarization and analysis and were designated as outliers. If feed consumption data (in g/day) were negative for a given dam and period, they were designated unrealistic and excluded from summarization and analysis. If feed consumption data for a given observational interval (e.g. gd 6-9, 9-12, 12-15 or 15-17) were designated outliers or unrealistic, then summarized data encompassing this period (e.g. treatment period) also did not include this value.

Result : Maternal toxicity observations:

In this study, inhalation of TAME by pregnant mice during gestation days 6-16 resulted in maternal toxicity at 3500 ppm, including maternal mortality (4 of 25), reductions in body weight, weight gain and treatment-related clinical signs of toxicity. The increased maternal absolute and relative liver weights at 1500 and 3500 ppm may have been due to induction of metabolizing enzymes and therefore increase in mass.

Maternal body weight was significantly reduced only at 3500 ppm for gd 15 and 17 (in-life and at termination). Prior to the start of exposures, maternal body weights were equivalent across all groups. Maternal weight change was significantly reduced at 3500 ppm for gd 9-12, 12-15, 15-17, 6-17 (exposure period) and 0-17 (entire gestation period). Maternal gestational weight change, corrected for the weight of the gravid uterus, was unaffected across groups. There were no effects on maternal weight change at 250 or 1500 ppm. Gravid uterine weight was significantly reduced at 3500 ppm. Maternal absolute liver weight was significantly increased at 1500 ppm but not at 3500 ppm, although the value at 3500 ppm was slightly increased. Maternal liver weight relative to weight at termination was significantly increased at 1500 and 3500 ppm. The increased relative liver weight may also have been due, in part, to the reduced body weights of the dams at termination at 3500 ppm.

Clinical observations related to TAME exposure at 3500 ppm included ataxia, hyperactivity, prone positioning, lethargy, gasping, rough coat, slow respiration, head tremors, squinted eyes, and maternal mortality. At 1500 ppm, dam exhibited half-closed eyes and head tremors. At 250 ppm, one dam delivered early on gd 16. In addition to solvent smell on fur, findings for the unscheduled deaths at 3500 ppm included red to dark red nail beds, red foci or red areas on lungs. These findings appeared to be consistent with severe congestion. There was clear indication of reduced pharmacological effects with time and maternal accommodation to the top two exposure concentrations. This interpretation was supported by observations of mortality at 3500 ppm early in the exposure period (gd 6-9) only and diminution over time in the incidence of clinical signs of toxicity, such as ataxia, lethargy, gasping and slow respiration. At scheduled necropsy, there were no gross findings in dams indicative of any lesions caused by the TAME exposure.

Maternal feed consumption (in g/day) was significantly reduced at 3500 ppm for gd 9-12, 12-15, 15-17, and 6-17 (exposure period). Maternal feed

consumption for the gestational period (gd 0-17) was unaffected across the other groups. At 1500 ppm, feed consumption was significantly reduced only for gd 6-9. When the data were expressed as g/kg/day, maternal feed consumption at 3500 ppm reduced only for gd 9-12. At 1500 ppm, feed consumption (as g/kg/day) was unaffected. There were no effects of treatment on maternal feed consumption at 250 ppm.

Embryo/fetal toxicity

There were no significant effects of maternal TAME vapor inhalation on gestational parameters, including number of ovarian corpora lutea, total number of uterine implantation sites, pre- or post-implantation loss, number of live fetuses per litter and gender ratio (% male fetuses) per litter. At 3500 ppm, there were significant increases in the percentage of late fetal deaths per litter and percentage of litters with late fetal deaths. There were significant concentration-related upward trends for percentage of non-live implants per litter and percentage of adversely affected (non-live plus malformed) implants per litter, with no significant pairwise comparisons with the concurrent control group values. Fetal body weight per litter when calculated as all fetuses, or males or females separately, was significantly reduced at 3500 ppm.

A statistically significant TAME-exposure-related increase was observed in the percentage of litters with fetal external malformations at 3500 ppm (31.68%); the value at 1500 ppm was also increased (18.28%) but not statistically significantly relative to the control group value (0.00%). A statistically significant, treatment-related increase was also observed in the percentage of litters with visceral variations at 3500 ppm (89.47%) relative to the control group value (47.83%). Values at 250 ppm (52.38%) and 1500 ppm (50.00%) were unchanged from the control group value. There were statistically significant, treatment-related upward trends ($P<0.001$) for the percentage of fetuses with variations per litter and for the percentage of male fetuses (but not for female fetuses) with variations per litter but no significant pairwise comparisons with the concurrent control group values for these parameters. The incidences of visceral, skeletal and total malformations and of external, skeletal and total variations were unchanged across groups when expressed as fetuses per litter or as litters with affected fetuses. External malformations were limited to cleft palate in three fetuses in three litters at 1500 ppm and 11 fetuses in six litters at 3500 ppm. One litter at 1500 ppm had three fetuses with polydactyly of fore- and hindpaws, one fetus with exencephaly and open left eye and one fetus with micrognathia and polydactyly. Fetal skeletal malformations were also distributed across all groups, with findings limited to the sternum (sternal plate and sternebrae) and ribs (branched, fused and inappropriate attachments of floating ribs to the sternum).

Fetal external variations were limited to hematomas in various locations at 250 and 1500 ppm. Fetal visceral variations were limited mainly to enlarged lateral ventricles of the cerebrum across all groups. One fetus in one litter at 0 ppm and three fetuses in three litters at 1500 ppm had red foci on urinary bladder and one fetus in one litter at 0 ppm had red foci on kidney. The incidence of enlarged lateral ventricles (full) and bilateral ventricles exhibited a clear treatment-related increased incidence only at 3500 ppm, with eight affected fetuses in seven litters at 0 ppm, six affected fetuses in four litters at 250 ppm, seven affected fetuses in seven litters at 1500 ppm and 38 affected fetuses in 16 litters at 3500 ppm. Fetal skeletal variations included extra rib(s) on lumbar vertebra no. 1 in all groups, misaligned sternebrae at 0, 250 and 1500 ppm, reduced ossification in sternebrae in all groups, in lumbar centrum at 1500 ppm and in thoracic centrum and pubis at 3500 ppm and floating extra rib cartilage at 1500 ppm.

Developmental toxicity was present at 3500 ppm, expressed specifically as increased incidence of late fetal deaths, reduced fetal body weights per litter and increased incidences of cleft palate (an external malformation) and of enlarged lateral ventricles of the cerebrum (a visceral variation). At 1500 ppm, three fetuses in three litters also exhibited cleft palate (with none observed at 250 of 9 ppm). This increase was not statistically significant, but it is considered biologically relevant and related to maternal TAME exposure. The finding of one additional litter at 1500 ppm with three multiply malformed fetuses (out of nine live fetuses total) may be unrelated to treatment because these malformations were not observed at 3500 ppm and were limited to only one litter at 1500 ppm. The observation of cleft palate in fetuses at 1500 and 3500 ppm appears to be consistent with a proposed mechanism for cleft palate in mice exposed to methyl tertiary butyl ether (MTBE). Maternal exposure to MTBE with anesthetic qualities at high concentrations associated with maternal stress results in elevated endogenous corticosteroid levels, which cause cleft palate in the developing offspring in mice (Bevan et al., 1997). Although those hormone levels were not determined in the present study, the biological mode of action of TAME appears to be similar and comparable to that of MTBE, as judged by clinical observations. At high exposure concentrations in mice, TAME exerts depressant effects on the central nervous system that resemble anesthetic properties and are preceded by a pronounced excitatory stage. Therefore, the brain stimulation and excitation may have induced a rise in endogenous corticosteroid levels in the mouse dams. The occurrence of a significantly increased incidence of fetal cleft palate at the 3500 ppm exposure level, coincident with maternal toxicity, suggests that stress of the dams is a contributing factor. Mice are sensitive to stress, and cleft palate occurs in offspring if the pregnant dams experience stress such as food and water deprivation, transportation, restraint or low humidity. That corticosteroids cause cleft palate in susceptible mouse strains is well documented.

The increased incidence of enlarged lateral ventricles of the fetal cerebrum at 3500 ppm is consistent with developmental delay because the fetuses at this exposure concentration exhibited mean body weights per litter of ca. 60% of the concurrent control group values. There were no notable developmental effects at 250 ppm. Almost all of the fetal malformations and variation findings observed in the present study are documented in control CD-1 mice fetuses collected at the Research Triangle Institute. In that historical database (47 control mouse litters with 589 fetuses), bilateral enlarged lateral ventricles was the most common fetal visceral variation in control fetuses.

Conclusion : TAME caused only unspecific embryotoxic effects that were apparently related to high exposure concentrations and associated concomitant maternal stress. The NOAEL for maternal and developmental toxicity in mice was 250 ppm in the present study.

Reliability : (1) valid without restriction
09.10.2006 (23)

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

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) American Petroleum Institute (1994). Tert-Amyl Methyl Ether (TAME) - Acute Toxicity to Daphnids (Daphnia magna) Under Flow-through Conditions. Toxicology Report Number 408. Springborn Laboratories, Inc. SLI Report 92-12-4545.

(2) American Petroleum Institute (1995). Closed-patch repeated insult dermal sensitization study of tertiary amyl methyl ether (TAME) in guinea pigs (Buehler Method). Project No. 403. Bio/dynamics Inc., East Laboratory, East Millstone, NJ, USA.

(3) American Petroleum Institute (1995). Tert-Amyl Methyl Ether (TAME) - Acute Toxicity to Rainbow Trout (Oncorhynchus mykiss) Under Flow-through Conditions. Toxicology Report Number 408. Springborn Laboratories, Inc. SLI Report 93-3-4682.

(4) American Petroleum Institute (1997). A 13-week inhalation toxicity/neurotoxicity study of tert-amyl methyl ether (TAME) in the rat and mouse via whole-body exposures with a 4-week recovery period. Project No. 95-6101. Huntingdon Life Sciences, East Millstone, NJ, USA.

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(6) Amoco (1991). Acute inhalation toxicity study of tert-amyl methyl ether (TAME) in rats. Project No. LO8100 1652. IIT Research Institute Life Sciences Research, Chicago, IL, USA.

(7) Bealing D (1995). Tertiary amyl methyl ether (TAME): assessment of ready biodegradability by measurement of oxygen uptake. Hazleton Europe. Report No. 1359/3-1018. 28 February 1995.

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10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

IUCLID

Data Set

Existing Chemical	:	ID: 142-82-5
CAS No.	:	142-82-5
EINECS Name	:	heptane
EC No.	:	205-563-8
TSCA Name	:	Heptane
Molecular Formula	:	C7H16

Producer related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	07.08.2006

Substance related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	07.08.2006
Status	:	
Memo	:	U.S. EPA - HPV Challenge Program
Printing date	:	01.10.2007
Revision date	:	
Date of last update	:	09.10.2006
Number of pages	:	28
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	**:**	

07.08.2006

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

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	:	= -90.6 °C
Sublimation	:	
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	other TS: heptane; (CAS #142-82-5)
Test substance	:	CAS #142-82-5; heptane; 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

07.08.2006 (11)

2.2 BOILING POINT

Value	:	= 98.4 °C at 1013 hPa
Decomposition	:	
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	other TS: heptane; (CAS #142-82-5)
Test substance	:	CAS #142-82-5; heptane; 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

07.08.2006 (11)

2.3 DENSITY

Type	:	density
Value	:	= .684 g/cm³ at 20 °C
Method	:	other: not specified
Year	:	
GLP	:	no data
Test substance	:	other TS: heptane; (CAS #142-82-5)
Test substance	:	CAS #142-82-5; heptane; 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

07.08.2006 (11)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	= 61.33 hPa at 25 °C
Decomposition	:	
Method	:	
Year	:	
GLP	:	no data
Test substance	:	other TS: heptane; (CAS #142-82-5)
Method	:	Method not specified.
Test substance	:	CAS #142-82-5; heptane; 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

07.08.2006 (3)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	= 4.5 at 25 °C
pH value	:	
Method	:	
Year	:	
GLP	:	no data
Test substance	:	other TS: heptane; (CAS #142-82-5)
Test substance	:	CAS #142-82-5; heptane; purity is unknown.
Reliability	:	(2) valid with restrictions The value cited by the author is a recommended value based on a review of data retrieved from the literature. This robust summary has a reliability rating of 2 because there is insufficient information available on the method.
Flag	:	Critical study for SIDS endpoint

07.08.2006 (14)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	= 3.4 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: no data
Year	:	
GLP	:	no data
Test substance	:	other TS: heptane; (CAS #142-82-5)
Test substance	:	CAS #142-82-5; heptane; purity is unknown.
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are from

a standard reference source.
Flag : Critical study for SIDS endpoint
07.08.2006 (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	:	= .00000000000687 cm³/(molecule*sec)
Degradation	:	= 50 % after 18.7 hour(s)
Deg. product	:	
Method	:	other (calculated): Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPI SuiteTM version 3.12
Year	:	
GLP	:	
Test substance	:	other TS: heptane; (CAS #142-82-5)
Method	:	Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPI SuiteTM 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	:	Heptane has the potential to volatilize to air, based on a relatively high vapor pressure, where it is subject to atmospheric oxidation. In air, heptane can react with photosensitized oxygen in the form of hydroxyl radicals (OH-). The computer program AOPWIN (atmospheric oxidation program for Microsoft Windows) (EPI SuiteTM, 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. Based on a 12-hour day, a rate constant of 6.87 E-12 cm3/molecule*sec, and an OH- concentration of 1.5 E6 OH-/cm3, heptane has a calculated half-life in air of 1.6 days or 18.7 hours of daylight.
Test substance	:	CAS #142-82-5; heptane; purity is unknown.
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

07.08.2006 (16)

Deg. product	:	
Method	:	
Year	:	
GLP	:	
Test substance	:	other TS: heptane; (CAS #142-82-5)
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, 1982).
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 and unsaturated hydrocarbons do not absorb light above 290 nm. Consequently, heptane is not subject to photolytic processes in the aqueous environment.

Test substance : CAS #142-82-5; heptane
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
07.08.2006 (8) (18)

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: heptane; (CAS #142-82-5)

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. Heptane is resistant to hydrolysis because it lacks a functional group that is hydrolytically reactive and Harris (1982) identifies hydrocarbons as generally resistant to hydrolysis. Therefore, hydrolysis will not contribute to the removal of heptane from the environment.
Test substance : CAS #142-82-5; heptane
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
07.08.2006 (6) (9)

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	100.21
Temperature	25° C
Log Kow	4.50
Water Solubility	3.4 g/m3
Vapor Pressure	6,133 Pa
Melting Point	-90.6° C

Result : Using the Mackay Level I calculation, the following distribution is predicted for heptane:

%Distribution	Compartment
99.91	Air
<0.01	Water
0.08	Soil
<0.01	Sediment
<0.01	Suspended Sediment
<0.01	Biota

Test substance : CAS #142-82-5; heptane
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
07.08.2006 (12)

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 cannot 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%	Emissions(kg/hr)
Air	26.0	1000
Water	48.5	1000
Soil	13.9	1000
Sediment	11.6	0

Test condition : Physicochemical data used in the calculation:

Parameter	Value w/ Units
Molecular Weight	100.21
Temperature	25° C
Log Kow	4.50
Water Solubility	3.4 g/m3
Vapor Pressure	6,133 Pa
Melting Point	-90.6° C

Reaction Half Lives in hours as predicted using EPI SuiteTM:

Air (gaseous)	35.9
Water (no susp. part.)	208
Bulk Soil	416
Bulk Sediment	1,870

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 : CAS #142-82-5; heptane

Conclusion : The majority of heptane is calculated to partition into the water phase, with smaller but significant amounts into air, soil, and sediment based on the modeling parameters used in this calculation. Heptane 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
07.08.2006 (13)

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type	:	aerobic
Inoculum	:	other: soil, non-adapted
Contact time	:	20 day(s)
Degradation	:	70 (±) % after 20 day(s)
Result	:	other: readily biodegradable
Deg. product	:	
Method	:	other: Standard Methods for the Examination of Water and Waste Water
Year	:	1971
GLP	:	no
Test substance	:	other TS: heptane; (CAS #142-82-5)
Result	:	70% degradation was measured after 20 days incubation with an unacclimated inoculum. % Biodegradation of test substance after days: 2 days = 28 % 5 days = 63 % 10 days = 70 % 20 days = 70 %
Test condition	:	American Public Health Association, Standard Methods for the Examination of Water and Waste Water, using 1.0 mg/l of test substance. Biodegradation was determined by measuring biological oxygen demand (BOD). Each 300 ml BOD bottle received 1.0 mg of heptane, 1.0 ml of a 1:10 suspension Hudson-Collamer silt loam soil in distilled water, and a mineral salts solution prepared as described in the test method. Bottles were incubated in the dark at 25C. The test substance was obtained from Aldrich Chemical Co.
Test substance	:	CAS #142-82-5; heptane; 99% pure.
Conclusion	:	Heptane is readily biodegradable.
Reliability	:	(2) valid with restrictions A standard test method was used. The study was conducted prior to GLP.

07.08.2006 (7)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

Species	:	other: see remark
Exposure period	:	at 25 °C
Concentration	:	
BCF	:	= 582
Elimination	:	
Method	:	other: calculation
Year	:	
GLP	:	no
Test substance	:	other TS: heptane; (CAS #142-82-5)
Remark	:	A log bioconcentration factor (BCF) of 2.77 is calculated (BCF = 582). With respect to a log Kow = 4.50, which was used to calculate the BCF, heptane

in the aquatic environment is expected to have a moderate potential to bioaccumulate.

Test substance : CAS #142-82-5; heptane

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

07.08.2006 (16)

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	
Species	:	other: fish
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	= .332
Method	:	other: ECOSAR version 0.99h, US EPA
Year	:	
GLP	:	
Test substance	:	other TS: heptane; (CAS #142-82-5)

Method : ECOSAR version 0.99h, U.S. 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	:	Calculated 96-hr LC50 for fish = 0.332 mg/L
Test condition	:	Experimental water solubility = 3.4 mg/l @ 25°C (Yalkowsky and Dannenfelser, 1992), log Kow = 4.50 @ 25°C (Sangster, 1989), and melting point = -90.6°C (Lide et al., 1997-1998) were entered into the program. Class: Neutral organics
Test substance	:	CAS #142-82-5; heptane
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated and not measured.

07.08.2006 (4)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	static
Species	:	other: Daphnia
Exposure period	:	48 hour(s)

Unit : mg/l
EC50 : = 1.5
Method : other: based on discussions in GESAMP/MARPOL meetings held in 1973
Year :
GLP : no data
Test substance : other TS: heptane; (CAS #142-82-5)

Method : Individual treatment concentrations were prepared by mixing the test substance in freshwater for 24 hours in a conical flask. The flask was almost completely filled with solution. After mixing, the treatment solutions were allowed to settle for 24 hours. The aqueous solution was then drained through a stopcock at the base of the flask and tested. Test vessels were 250 ml conical flasks with 25 daphnids per flask. Two replicates of each treatment level and control were evaluated.

Organisms supplied by testing lab; age = <24 hours old; parents age = approximately 21 days old.
Statistical method:
Parametric model developed by Kooijman (Kooijman, S.A.L.M. 1981. Parametric analyses of mortality rate in bio-assays. Water Res., 15:107-119.).

Result : 48-hr EC50 for a daphnid = 0.423 mg/L
Test condition : Dissolved oxygen was >50% saturation during the study. The pH was 7.5 to 8.3. Temperature was 20 Deg C.

Analytical method used was Gas Chromatography with Flame Ionization Detection (GC-FID). Nominal treatment levels ranged from 0.32 to 10 mg/L. Only the following analytical data were reported:

Nominal Conc. (mg/L)	Initial Measured Conc. (mg/L)	48-hr Measured Conc. (mg/L)
0.32	0.04	Not Determined
1.0	0.04	Not Determined
3.2	0.5	Not Determined
5.6	2.1	1.7
10	2.2	Not Determined

Test substance : CAS #142-82-5; heptane
Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because there is less raw data and information on the testing procedure than is desirable in order to rate this study for reliability at a level higher than 2. There is sufficient information in the report to suggest that the testing procedure generally followed an acceptable test guideline, OECD 202, and used acceptable methods to prepare exposure solutions.
Flag : Critical study for SIDS endpoint
07.08.2006 (15)

Type : semistatic
Species : other: Gammarid (Chaetogammarus marinus)
Exposure period : 96 hour(s)
Unit : mg/l
LC50 : = .2
Method : other: Static Gammarid Acute Toxicity Test
Year :
GLP : no data
Test substance : other TS: heptane; (CAS #142-82-5)

Method : Individual treatment solutions were prepared by mixing the test substance in freshwater for 24 hours in conical flasks. The flask was almost completely filled with solution. After mixing, the treatment solutions were allowed to settle for 24 hours. The aqueous solution was then drained through a stopcock at the base of the flask and tested. Test vessels were

scintillation vials almost filled with approximately 20 ml of test solution and one organism per vial. Ten organisms were tested per treatment level. Organisms were transferred into fresh control and test solutions every 24 hours up to 96 hours.

Organisms supplied by testing lab, grown in natural seawater with a salinity of 2.8%; length = 5 mm.
Statistical method:
Parametric model developed by Kooijman (Kooijman, S.A.L.M. 1981. Parametric analyses of mortality rate in bio-assays. Water Res., 15:107-119.).

Result : 96-hr LC50 for a gammarid = 0.2 mg/L

Test condition : Dissolved oxygen was >50% saturation during the study. The pH was 7.5 to 8.3. Temperature was 15 Deg C. Natural seawater was used with a salinity of 2.8%

Analytical method used was Gas Chromatography with Flame Ionization Detection (GC-FID). Nominal treatment levels ranged from 0.32 to 10 mg/L. Test solutions were analyzed only upon test initiation.

Only the following analytical data were reported:

Nominal Conc. (mg/L)	Initial Measured Conc. (mg/L)
0.32	0.003
1.0	0.07
3.2	0.2
5.6	Not Determined
10	Not Determined

Test substance : CAS #142-82-5; heptane

Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because there is less raw data and information on the testing procedure than is desirable in order to rate this study for reliability at a level higher than 2. There is sufficient information in the report to suggest that the testing procedure generally followed an acceptable test guideline and used acceptable methods to prepare exposure solutions.

Flag : Critical study for SIDS endpoint

07.08.2006 (15)

Type : semistatic

Species : other: mysid shrimp (Mysidopsis bahia)

Exposure period : 96 hour(s)

Unit : mg/l

LC50 : = .1

Method : other: Static Gammarid Acute Toxicity Test

Year :

GLP : no data

Test substance : other TS: heptane; (CAS #142-82-5)

Method : Individual treatment solutions were prepared by mixing the test substance in freshwater for 24 hours in conical flasks. The flask was almost completely filled with solution. After mixing, the treatment solutions were allowed to settle for 24 hours. The aqueous solution was then drained through a stopcock at the base of the flask and tested. Test vessels were scintillation vials almost filled with approximately 20 ml of test solution and one organism per vial. Ten organisms were tested per treatment level. Organisms were transferred into fresh control and test solutions every 24 hours up to 96 hours.

Organisms supplied by testing lab, grown in natural seawater with a salinity of 2.8%; test organisms were approximately 4 weeks old, with lengths of

approximately 6 mm.
Statistical method:
Parametric model developed by Kooijman (Kooijman, S.A.L.M. 1981. Parametric analyses of mortality rate in bio-assays. Water Res., 15:107-119.).

Result : 96-hr LC50 for a gammarid = 0.1 mg/L

Test condition : Dissolved oxygen was >50% saturation during the study. The pH was 7.5 to 8.3. Temperature was 20 Deg C. Natural seawater was used with a salinity of 2.8%

Analytical method used was Gas Chromatography with Flame Ionization Detection (GC-FID). Nominal treatment levels ranged from 0.32 to 10 mg/L. Test solutions were analyzed only upon test initiation.

Only the following analytical data were reported:

Nominal Conc. (mg/L)	Initial Measured Conc. (mg/L)
0.32	0.003
1.0	0.07
3.2	0.2
5.6	Not Determined
10	Not Determined

Test substance : CAS #142-82-5; heptane

Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because there is less raw data and information on the testing procedure than is desirable in order to rate this study for reliability at a level higher than 2. There is sufficient information in the report to suggest that the testing procedure generally followed an acceptable test guideline and used acceptable methods to prepare exposure solutions.

Flag : Critical study for SIDS endpoint

07.08.2006 (15)

Type :

Species : other: Daphnia

Exposure period : 48 hour(s)

Unit : mg/l

LC50 : = .423

Method : other: ECOSAR version 0.99h, US EPA

Year :

GLP :

Test substance : other TS: heptane; (CAS #142-82-5)

Method : ECOSAR version 0.99h, U.S. 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 : Calculated 48-hr LC50 for a dahpnid = 0.423 mg/L

Test condition : Experimental water solubility = 3.4 mg/l @ 25°C (Yalkowsky and Dannenfelser, 1992), log Kow = 4.50 @ 25°C (Sangster, 1989), and melting point = -90.6°C (Lide et al., 1997-1998) were entered into the program.
Class: Neutral organics

Test substance : CAS #142-82-5; heptane

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

07.08.2006 (4)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species : other algae: Green Alga

Endpoint :

Exposure period : 96 hour(s)

Unit : mg/l

EC50 : = .305

ChV : = .129

Method : other: ECOSAR version 0.99h, US EPA

Year :

GLP :

Test substance : other TS: heptane; (CAS #142-82-5)

Method : ECOSAR version 0.99h, U.S. 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	:	Calculated 96-hr EC50 for a green alga = 0.305 mg/L Calculated 96-hr ChV for a green alga = 0.129 mg/L
Test condition	:	Experimental water solubility = 3.4 mg/l @ 25°C (Yalkowsky and Dannenfelser, 1992), log Kow = 4.50 @ 25°C (Sangster, 1989), and melting point = -90.6°C (Lide et al., 1997-1998) were entered into the program. Class: Neutral organics
Test substance	:	CAS #142-82-5; heptane
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated and not measured.

07.08.2006 (4)

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

5.1.2 ACUTE INHALATION TOXICITY

Type	:	LC50
Value	:	> 29.29 mg/l
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male/female
Number of animals	:	10
Vehicle	:	other: none
Doses	:	29.29 mg/L (17940 ppm)
Exposure time	:	4 hour(s)
Method	:	other: Similar to OECD guideline 403
Year	:	1982
GLP	:	
Test substance	:	other TS: n-Heptane (CAS # 142-82-5)
Remark	:	Animals were exposed to n-heptane vapor for 4 hours at a concentration of 29.29 mg/L (nominal) or 17937.5 ppm (mean analytical).
Result	:	There was no mortality during the course of the study. A slight reduction of mean male body weights was noted on day 2 post exposure but males recovered by day 4. All animals appeared normal throughout the study and at terminal necropsy with the exception of one female observed with enlarged mandibular lymph nodes on the right side.
Conclusion	:	n-Heptane has a low order of toxicity by the inhalation route of exposure.
Reliability	:	(2) valid with restrictions

09.10.2006 (10)

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

Type	:	
Species	:	rat
Sex	:	male/female
Strain	:	Sprague-Dawley

Route of admin.	:	inhalation
Exposure period	:	6 hours/day
Frequency of treatm.	:	5 days/week for 26 weeks
Post exposure period	:	2-week post exposure recovery period
Doses	:	0, 500, 2000 and 4000 ppm
Control group	:	yes
NOAEL	:	= 2970 ppm
Method	:	other: similar to OECD guideline 413
Year	:	1980
GLP	:	
Test substance	:	other TS: n-Heptane (CAS # 142-82-5)
Remark	:	Animals were exposed to 0, 398 or 2970 ppm n-heptane. Type: 26-week inhalation toxicity study Number of animals: 15/sex/dose group
Result	:	There were no treatment-related deaths during the study. The only treatment-related observations were labored breathing or rapid breathing and slight prostration during the first week of study during exposure only, and anogenital fur and dry rales during weekly observations. The in chamber signs were generally more numerous and severe in the higher dose group and appeared to abate by the second week of the study. No treatment-related effects were observed for body weight, hematology or urinalysis. Serum alkaline phosphatase was significantly elevated in female high dose rats and slightly elevated in low dose females. All other clinical chemistry values appeared normal with the exception of one male high level rat whose serum glutamic pyruvic transaminase and serum alkaline phosphatase levels were markedly elevated when compared to all other male rats on test. Proteinuria, elevated specific gravity and ketones were observed but do not appear to be related to treatment.
Conclusion	:	The effects observed are consistent with acute CNS depression and generally abated by the second week of study. Under the conditions of this study, the LOAEL for acute CNS depression is 2,970 ppm and the NOAEL for systemic toxicity is 2,970 ppm.
Reliability	:	(2) valid with restrictions

09.10.2006 (1)

Type	:	
Species	:	rat
Sex	:	male
Strain	:	Sprague-Dawley
Route of admin.	:	inhalation
Exposure period	:	9 hours/day
Frequency of treatm.	:	5 days/week for 7, 14 or 30 weeks
Post exposure period	:	None. Animals were sacrificed at 7, 14 or 30 weeks.
Doses	:	0, 1500 ppm
Control group	:	other: yes, omitted the second air flow
NOAEL	:	> 1500 - ppm
Method	:	other: none specified
Year	:	1981
GLP	:	
Test substance	:	other TS: n-Heptane (CAS # 142-82-5)
Remark	:	Only males and one dose group were used. The primary objective of this study was to assess the appearance of polyneuropathy and urinary metabolites in rats following exposure to analytical grade solvents frequently used in Italian shoe factories. Nerve tissue was examined microscopically. Body weights were analyzed by a two-way analysis of variance and Student's t test for the comparison of two slopes. Type: 30-week inhalation neurotoxicity study

Number of animals: 6-9 males/dose group

Result : None of the animals developed signs of neuropathy. There were no differences in weight gain of rats (30 weeks) compared to controls. Differences between mean values for hindlimb spreads observed in treated animals and controls were not statistically significant. However, authors note that in their hands, the test employed turned out to be scarcely effective due to high individual variability. No histological signs of giant axonal degeneration were noted in rats treated at 1500 ppm (30 weeks).

Conclusion : Under the conditions of this test, inhalation of n-heptane at 1500 ppm did not induce neuropathy in rats.

Reliability : (2) valid with restrictions

09.10.2006 (5)

5.5 GENETIC TOXICITY 'IN VITRO'

Type : Bacterial reverse mutation assay
System of testing : Salmonella typhimurium and Escherichia coli
Test concentration : Doses ranging from 3.91 to 250 ug/ml
Cycotoxic concentr. : 500 µg/ml
Metabolic activation : with and without
Result : negative
Method : other: No specific method or guideline was noted.
Year : 1982
GLP :
Test substance : other TS: heptane (CAS # 142-82-5)

Remark : GLP: Quality assurance statement
Strains tested: Salmonella typhimurium tester strains TA98, TA100, TA1535, TA1537, TA1538; Escherichia coli strains WP2, WP uvr A

Test substance concentrations: 3.91, 7.81, 15.6, 31.3, 62.5, 125, 250 mg/ml

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

Vehicle: Tween 80/ethanol

Positive Controls: benzo[a]pyrene, 4-nitroquinoline-N-oxide, sodium azide, neutral red, potassium dichromate.

Cytotoxicity study: A toxicity screening test conducted prior to the full assay indicated cytotoxicity at 500 mg/ml with and without metabolic activation.

The cultures were incubated at 37°C for 48-72 hours in a sealed container before the revertant colonies were counted. Pre-incubation method was used to limit evaporation of test material.

Result : The addition of heptane at amounts up to 250 mg per ml to cultures of Escherichia coli WP2 and WP2 uvr A, Salmonella typhimurium TA 1535, TA 1537, TA 1538, TA 98, and TA 100 did not lead to an increase in the reverse gene mutation frequency in any of these strains, either in the presence or in the absence of rat liver S9 fraction. In one assay with Escherichia coli WP2 in the presence of S9 fraction a greater than 2.5 fold increase over control values was seen at 15.6 and 31.3 mg per ml. This increase was not dose-related nor repeated in replicate assays and was therefore not considered to be a compound-related effect.

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

Reliability : (1) valid without restriction

09.10.2006 (2)

Type	:	other: Mitotic gene conversion assay
System of testing	:	Yeast
Test concentration	:	Doses ranging from 0.01 to 5.0 mg/ml
Cycotoxic concentr.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	other: No specific method or guideline was noted
Year	:	1982
GLP	:	
Test substance	:	other TS: heptane (CAS # 142-82-5)
Remark	:	GLP: Quality assurance statement Strains tested: Saccharomyces cerevisiae JD1 Test substance concentrations: 0.01, 0.1, 0.5, 1.0, 5.0 mg/ml Metabolic activation: With and without (S9 fraction mix of livers from Aroclor 1254 pretreated rats) Vehicle: Tween 80/ethanol Positive Controls: 4-nitroquinoline-N-oxide, cyclophosphamide After 18-hour incubation at 30°C the cultures were placed onto the appropriate culture media for the selection of prototrophic colonies. After three days incubation at 30°C the numbers of prototrophic colonies were counted.
Result	:	Exposure of Saccharomyces cerevisiae JD1 to heptane at concentrations up to 5.0 mg/ml did not result in a consistent increase in the rate of mitotic gene conversion, either in the presence or in the absence of rat liver S9 fraction.
Conclusion	:	Under the conditions of this study, the test material was not genotoxic.
Reliability	:	(1) valid without restriction

09.10.2006 (2)

Type	:	other: Chromosome aberration assay
System of testing	:	Rat Liver (RL4) cells
Test concentration	:	2.5, 5, 10 ug/ml
Cycotoxic concentr.	:	20 ug/ml (100% cytotoxicity), 10 ug/ml (0% cytotoxicity)
Metabolic activation	:	
Result	:	negative
Method	:	other: No specific method or guideline was noted
Year	:	1982
GLP	:	
Test substance	:	other TS: heptane (CAS # 142-82-5)
Remark	:	GLP: Quality assurance statement Vehicle: Tween 80/ethanol Positive Controls: 7,12-Dimethylbenzanthracene (DMBA) Cultured rat liver cells were grown and treated on glass microscopic slides contained in 100-ml volume glass Leighton tubes. After 22-hour exposure to test compound or vehicle, colcemid was added to each culture. After further 2 hours, the slides were removed, subjected to hypotonic treatment followed by fixation (methanol:acetic acid, 3:1) and stained with Giemsa. The preparations were randomly coded and 100 cells from each culture were analyzed microscopically.
Result	:	In one culture exposed to 10 mg/ml of heptane a total of 7 chromatid gaps were seen; this increased the frequency to 0.024 gaps per cell which, although greater than the vehicle control frequency, was not accompanied

by an increase in any other type of aberration and is not considered to be a compound-related effect. Thus there was no significant or dose-related increase of chromosome damage in any of the culture exposed to heptane. Cultures exposed to the positive control material, DMBA, showed a marked increase in the frequency of chromosome damage.

Conclusion : Under the conditions of this study, the test material was not clastogenc.
Reliability : (2) valid with restrictions
09.10.2006 (2)

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

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

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10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

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EOR
F001 483
F002 3.1.1
F003 8
F004 A37-009
EOR
F001 483
F002 3.1.1
F003 9
F004 A37-009
EOR
F001 483
F002 3.1.2
F003 2
F004 A37-009
EOR
F001 483
F002 3.3.1
F003 3
F004 A37-009
EOR
F001 483
F002 3.3.1
F003 4
F004 A37-009
EOR
F001 483
F002 3.7
F003 2
F004 A37-009
EOR
F001 483
F002 4.2
F003 3
F004 A37-009
EOR
F001 483
F002 4.2
F003 4
F004 A37-009
EOR
F001 483
F002 4.2

F003 5
F004 A37-009
EOB
C
B051 DS_COMPONENT_TAB
F001 483
F002 0
F003 142-82-5
F012 N
F010 07-08-2006
F004 12032693
F005 07-08-2006
F006 12032693
F007 07-08-2006
F008 U.S. EPA - HPV Challenge Program
F009 A35-02
EOR
F001 483
F002 1
F003 142-82-5
F012 N
F010 17-08-1999
F004 12029804
F005 01-08-1999
F006 12029804
F007 01-08-1999
F008 Hydrocarbon Consortium Iuclid
F009 A35-02
EOB
C
B101 GI_GENERAL_INFORM_TAB
F001 483
F002 1
F003 07-08-2006
F004 CLGETTS1
F013 1
F010 A04-04
F011 A19-02
EOB
C
B201 PC_MELTING_TAB
F001 483
F002 1
F003 07-08-2006
F004 CLGETTS1
F015 A36-003
F016 1
F007 A02-03
F008 -90.6
F012 P01-03: not specified
F014 A03-02
F020 A01-03: heptane; (CAS #142-82-5)

EOB
C
B202 PC_BOILING_TAB
F001 483
F002 1
F003 07-08-2006
F004 CLGETTS1
F016 A36-003
F017 1
F007 A02-03
F008 98.4
F010 1013
F011 P02-01
F013 P03-03: not specified
F015 A03-02
F018 A01-03: heptane; (CAS #142-82-5)
EOB
C
B203 PC_DENSITY_TAB
F001 483
F002 1
F003 07-08-2006
F004 CLGETTS1
F016 A36-003
F017 1
F007 P05-02
F008 A02-03
F009 .684
F011 P18-01
F012 20
F013 P04-03: not specified
F015 A03-02
F018 A01-03: heptane; (CAS #142-82-5)
EOB
C
B204 PC_VAPOUR_TAB
F001 483
F002 1
F003 07-08-2006
F004 CLGETTS1
F015 A36-003
F016 1
F007 A02-03
F008 61.33
F010 P02-01
F011 25
F014 A03-02
F018 A01-03: heptane; (CAS #142-82-5)
EOB
C
B205 PC_PARTITION_TAB
F001 483

F002 1
F003 07-08-2006
F004 CLGETTS1
F014 A36-003
F015 1
F007 A02-03
F008 4.5
F010 25
F013 A03-02
F016 A01-03: heptane; (CAS #142-82-5)
F020 C15-001
EOB
C
B206 PC_WATER_SOL_TAB
F001 483
F002 1
F003 07-08-2006
F004 CLGETTS1
F023 A36-003
F024 1
F007 A02-03
F008 P08-02
F009 3.4
F011 25
F020 P09-03: no data
F022 A03-02
F025 A01-03: heptane; (CAS #142-82-5)
F030 C14-001
EOB
C
B301 EN_PHOTODEGRADATION_TAB
F001 483
F002 8
F003 07-08-2006
F004 CLGETTS1
F045 A36-003
F046 1
F007 A01-03: heptane; (CAS #142-82-5)
F008 F01-01
F009 F02-05: Calculated values using AOPWIN version 1.89, a subroutine of the
* computer program EPI SuiteTM version 3.12
F023 25
F034 F06-03
F035 1500000
F036 F07-02
F044 A02-03
F037 .00000000000687
F038 A02-03
F040 50
F041 18.7
F042 F05-02
EOR

F001 483
F002 9
F003 07-08-2006
F004 CLGETTS1
F045 A36-003
F046 2
F007 A01-03: heptane; (CAS #142-82-5)
EOB
C
B302 EN_STABILITY_IN_WATER_TAB
F001 483
F002 2
F003 07-08-2006
F004 CLGETTS1
F040 A36-003
F041 1
F007 A01-03: heptane; (CAS #142-82-5)
F008 F08-01
F009 F09-03: Technical discussion
F039 A03-02
EOB
C
B305 EN_TRANSPORT_TAB
F001 483
F002 3
F003 07-08-2006
F004 CLGETTS1
F011 A36-003
F012 1
F008 F22-01: air - biota - sediment(s) - soil - water
F009 F21-01: Calculation according Mackay, Level I
EOR
F001 483
F002 4
F003 07-08-2006
F004 CLGETTS1
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
C
B308 EN_BIODEGRADATION_TAB
F001 483
F002 4
F003 07-08-2006
F004 CLGETTS1
F047 A36-003
F048 1
F007 A01-03: heptane; (CAS #142-82-5)

F008 F25-01
F009 F26-25: Standard Methods for the Examination of Water and Waste Water
F010 1971
F011 F27-0166: soil, non-adapted
F017 70
F018 20
F019 F05-01
F020 F30-02: readily biodegradable
F046 A03-01
F052 20
F053 F05-01
EOB
C
B310 EN_BIOACCUMULATION_TAB
F001 483
F002 2
F003 07-08-2006
F004 CLGETTS1
F021 A36-003
F022 1
F007 A01-03: heptane; (CAS #142-82-5)
F008 E02-0161: see remark
F009 F34-06: calculation
F015 25
F016 A02-03
F017 582
F020 A03-01
EOB
C
B401 EC_FISHTOX_TAB
F001 483
F002 5
F003 07-08-2006
F004 CLGETTS1
F033 A36-003
F034 1
F007 A01-03: heptane; (CAS #142-82-5)
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 .332
EOB
C
B402 EC_DAPHNIATOX_TAB
F001 483
F002 3
F003 07-08-2006
F004 CLGETTS1
F032 A36-003

F033 1
F007 A01-03: heptane; (CAS #142-82-5)
F008 E06-0034: Daphnia
F009 E07-04: based on discussions in GESAMP/MARPOL meetings held in 1973
F011 48
F012 E04-02
F013 E05-02
F020 A02-03
F021 1.5
F031 A03-02
F042 E01-05
EOR
F001 483
F002 4
F003 07-08-2006
F004 CLGETTS1
F032 A36-003
F033 2
F007 A01-03: heptane; (CAS #142-82-5)
F008 E06-0034: Gammarid (Chaetogammarus marinus)
F009 E07-04: Static Gammarid Acute Toxicity Test
F011 96
F012 E04-02
F013 E05-02
F026 LC50
F027 A02-03
F028 .2
F031 A03-02
F042 E01-04
EOR
F001 483
F002 5
F003 07-08-2006
F004 CLGETTS1
F032 A36-003
F033 3
F007 A01-03: heptane; (CAS #142-82-5)
F008 E06-0034: mysid shrimp (Mysidopsis bahia)
F009 E07-04: Static Gammarid Acute Toxicity Test
F011 96
F012 E04-02
F013 E05-02
F026 LC50
F027 A02-03
F028 .1
F031 A03-02
F042 E01-04
EOR
F001 483
F002 6
F003 07-08-2006
F004 CLGETTS1

F032 A36-003
F033 4
F007 A01-03: heptane; (CAS #142-82-5)
F008 E06-0034: Daphnia
F009 E07-04: ECOSAR version 0.99h, US EPA
F011 48
F012 E04-02
F013 E05-02
F026 LC50
F027 A02-03
F028 .423
EOB
C
B403 EC_ALGAETOX_TAB
F001 483
F002 2
F003 07-08-2006
F004 CLGETTS1
F036 A36-003
F037 1
F007 A01-03: heptane; (CAS #142-82-5)
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 .305
F030 ChV
F031 A02-03
F032 .129
EOB
C
B502 TO_ACUTE_INHAL_TAB
F001 483
F002 1
F003 09-10-2006
F004 CLGETTS1
F019 A36-003
F020 1
F007 A01-03: n-Heptane (CAS # 142-82-5)
F008 T05-03
F009 T02-24
F010 T06-03: Similar to OECD guideline 403
F011 1982
F012 A02-04
F013 29.29
F015 T07-01
F016 4
F017 T08-01
F021 T24-03
F022 10

F023 T52-003: none
F024 T23-42
F025 29.29 mg/L (17940 ppm)
EOB
C
B508 TO_REPEATED_DOSE_TAB
F001 483
F002 1
F003 09-10-2006
F004 CLGETTS1
F030 A36-003
F031 1
F007 A01-03: n-Heptane (CAS # 142-82-5)
F008 T02-24
F009 T23-42
F010 T24-03
F011 T25-08
F012 T26-16: similar to OECD guideline 413
F013 1980
F014 6 hours/day
F015 5 days/week for 26 weeks
F016 2-week post exposure recovery period
F017 0, 500, 2000 and 4000 ppm
F018 T27-07
F019 A02-03
F020 2970
F022 T28-05
EOR
F001 483
F002 2
F003 09-10-2006
F004 CLGETTS1
F030 A36-003
F031 2
F007 A01-03: n-Heptane (CAS # 142-82-5)
F008 T02-24
F009 T23-42
F010 T24-02
F011 T25-08
F012 T26-16: none specified
F013 1981
F014 9 hours/day
F015 5 days/week for 7, 14 or 30 weeks
F016 None. Animals were sacrificed at 7, 14 or 30 weeks.
F017 0, 1500 ppm
F018 T27-03: yes, omitted the second air flow
F019 A02-04
F020 1500
F022 T28-05
EOB
C
B509 TO_GENETIC_IN_VITRO_TAB

F001 483
F002 1
F003 09-10-2006
F004 CLGETTS1
F016 A36-002
F017 1
F007 A01-03: heptane (CAS # 142-82-5)
F008 T30-05
F009 T31-18: No specific method or guideline was noted.
F010 1982
F011 Salmonella typhimurium and Escherichia coli
F012 T32-03
F013 T33-02
F015 Doses ranging from 3.91 to 250 ug/ml
F018 500 µg/ml
EOR
F001 483
F002 2
F003 09-10-2006
F004 CLGETTS1
F016 A36-002
F017 2
F007 A01-03: heptane (CAS # 142-82-5)
F008 T30-19: Mitotic gene conversion assay
F009 T31-18: No specific method or guideline was noted
F010 1982
F011 Yeast
F012 T32-03
F013 T33-02
F015 Doses ranging from 0.01 to 5.0 mg/ml
EOR
F001 483
F002 3
F003 09-10-2006
F004 CLGETTS1
F016 A36-003
F017 3
F007 A01-03: heptane (CAS # 142-82-5)
F008 T30-19: Chromosome aberration assay
F009 T31-18: No specific method or guideline was noted
F010 1982
F011 Rat Liver (RL4) cells
F013 T33-02
F015 2.5, 5, 10 ug/ml
F018 20 ug/ml (100% cytotoxicity), 10 ug/ml (0% cytotoxicity)
EOB
C
B601 TEXT_TAB
F002 483
F010 2.1
F004 1
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 258882
EOR
F002 483
F010 2.1
F004 1
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 258881
EOR
F002 483
F010 2.1
F004 1
F005 TS
F006 CAS #142-82-5; heptane; purity is unknown.
F007 CAS #142-82-5; heptane; purity is unknown.
F020 258880
EOR
F002 483
F010 2.2
F004 1
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 258885
EOR
F002 483
F010 2.2
F004 1
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 258884
EOR
F002 483
F010 2.2
F004 1
F005 TS

F006 CAS #142-82-5; heptane; purity is unknown.
F007 CAS #142-82-5; heptane; purity is unknown.
F020 258883
EOR
F002 483
F010 2.3
F004 1
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 258888
EOR
F002 483
F010 2.3
F004 1
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 258887
EOR
F002 483
F010 2.3
F004 1
F005 TS
F006 CAS #142-82-5; heptane; purity is unknown.
F007 CAS #142-82-5; heptane; purity is unknown.
F020 258886
EOR
F002 483
F010 2.4
F004 1
F005 ME
F006 Method not specified.
F007 Method not specified.
F020 258890
EOR
F002 483
F010 2.4
F004 1
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 258892
EOR
F002 483
F010 2.4
F004 1
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 258891
EOR
F002 483
F010 2.4
F004 1
F005 TS
F006 CAS #142-82-5; heptane; purity is unknown.
F007 CAS #142-82-5; heptane; purity is unknown.
F020 258889
EOR
F002 483
F010 2.5
F004 1
F005 RE
F006 Sangster, J (1989). Octanol-water partition coefficients of simple
* organic compounds. J Phys Chem Ref Data 18:1111-1227.
F007 Sangster, J (1989). Octanol-water partition coefficients of simple
* organic compounds. J Phys Chem Ref Data 18:1111-1227.
F020 258895
EOR
F002 483
F010 2.5
F004 1
F005 RL
F006 The value cited by the author is a recommended value based on a review of
* data retrieved from the literature. This robust summary has a reliability
* rating of 2 because there is insufficient information available on the
* method.
F007 The value cited by the author is a recommended value based on a review of
* data retrieved from the literature. This robust summary has a reliability
* rating of 2 because there is insufficient information available on the
* method.
F020 258894
EOR
F002 483
F010 2.5
F004 1
F005 TS

F006 CAS #142-82-5; heptane; purity is unknown.
F007 CAS #142-82-5; heptane; purity is unknown.
F020 258893
EOR
F002 483
F010 2.6.1
F004 1
F005 RE
F006 Yalkowsky S and Dannenfelser R (1992). Aquasol Database of Aqueous
* Solubility. Version 5. College of Pharmacy, University of Arizona, AZ,
* USA.
F007 Yalkowsky S and Dannenfelser R (1992). Aquasol Database of Aqueous
* Solubility. Version 5. College of Pharmacy, University of Arizona, AZ,
* USA.
F020 258898
EOR
F002 483
F010 2.6.1
F004 1
F005 RL
F006 This robust summary has a reliability rating of 2 because the data are
* from a standard reference source.
F007 This robust summary has a reliability rating of 2 because the data are
* from a standard reference source.
F020 258897
EOR
F002 483
F010 2.6.1
F004 1
F005 TS
F006 CAS #142-82-5; heptane; purity is unknown.
F007 CAS #142-82-5; heptane; purity is unknown.
F020 258896
EOR
F002 483
F010 3.1.1
F004 8
F005 ME
F006 Calculated values using AOPWIN version 1.89, a subroutine of the computer
* program EPI SuiteTM version 3.12
**
** Indirect photodegradation, or atmospheric oxidation potential, is based
* on the structure-activity relationship methods developed by
F007 Calculated values using AOPWIN version 1.89, a subroutine of the computer
* program EPI SuiteTM 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 258899
EOR
F002 483
F010 3.1.1
F004 8
F005 RE
F006 U.S. Environmental Protection Agency (U.S. EPA) (2000). EPI SuiteTM,
* Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.
F007 U.S. Environmental Protection Agency (U.S. EPA) (2000). EPI SuiteTM,
* Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.
F020 258903
EOR
F002 483
F010 3.1.1
F004 8
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 258902
EOR
F002 483
F010 3.1.1
F004 8
F005 RM
F006 Heptane has the potential to volatilize to air, based on a relatively
* high vapor pressure, where it is subject to atmospheric oxidation. In
* air, heptane can react with photosensitized oxygen in the form of
* hydroxyl radicals
** (OH-). The compu
F007 Heptane has the potential to volatilize to air, based on a relatively
* high vapor pressure, where it is subject to atmospheric oxidation. In
* air, heptane can react with photosensitized oxygen in the form of
* hydroxyl radicals
** (OH-). The computer program AOPWIN (atmospheric oxidation program for
* Microsoft Windows) (EPI SuiteTM, 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.
** Based on a 12-hour day, a rate constant of 6.87 E-12 cm3/molecule*sec,
* and an OH- concentration of 1.5 E6 OH-/cm3, heptane has a calculated
* half-life in air of 1.6 days or 18.7 hours of daylight.
F020 258900
EOR
F002 483
F010 3.1.1
F004 8
F005 TS

F006 CAS #142-82-5; heptane; purity is unknown.
F007 CAS #142-82-5; heptane; purity is unknown.
F020 258901
EOR
F002 483
F010 3.1.1
F004 9
F005 ME
F006 Technical discussion
F007 Technical discussion
F020 258904
EOR
F002 483
F010 3.1.1
F004 9
F005 RE
F006 Harris J (1982). Rate of Aqueous Photolysis. In: Handbook of Chemical
* Property Estimation Methods. Chapter 8. Edited by WJ Lyman, WF Reehl and
* DH Rosenblatt. McGraw-Hill Book Company, New York, NY, USA.
F007 Harris J (1982). Rate of Aqueous Photolysis. In: Handbook of Chemical
* Property Estimation Methods. Chapter 8. Edited by WJ Lyman, WF Reehl and
* DH Rosenblatt. McGraw-Hill Book Company, New York, NY, USA.
F020 258908
EOR
F002 483
F010 3.1.1
F004 9
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 258909
EOR
F002 483
F010 3.1.1
F004 9
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 258907
EOR
F002 483
F010 3.1.1
F004 9
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, 1982).
** 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 and unsaturated
* hydrocarbons do not absorb light above 290 nm. Consequently, heptane is
* not subject to photolytic processes in the aqueous environment.
F020 258905
EOR
F002 483
F010 3.1.1
F004 9
F005 TS
F006 CAS #142-82-5; heptane
F007 CAS #142-82-5; heptane
F020 258906
EOR
F002 483
F010 3.1.2
F004 2
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 258913
EOR
F002 483
F010 3.1.2
F004 2
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 258914
EOR
F002 483
F010 3.1.2
F004 2
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 258912
EOR
F002 483
F010 3.1.2
F004 2
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. Heptane is resistant to hydrolysis because it lacks a
* functional group that is hydrolytically reactive and Harris (1982)
* identifies hydrocarbons as generally resistant to hydrolysis. Therefore,
* hydrolysis will not contribute to the removal of heptane from the
* environment.
F020 258910
EOR
F002 483
F010 3.1.2
F004 2
F005 TS
F006 CAS #142-82-5; heptane
F007 CAS #142-82-5; heptane
F020 258911
EOR
F002 483
F010 3.3.1
F004 3
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 258919
EOR
F002 483
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 258918
EOR
F002 483
F010 3.3.1
F004 3
F005 RM
F006 Physicochemical data used in the calculation:
**
** Parameter Value w/ Units
** Molecu 100.21
** Temperature 25° C
** Log Kow 4.5
** Water S 3.4 g/m3
** Vapor Pressure 6,133 Pa
** Melting Point -90.6° C
F007 Physicochemical data used in the calculation:
**
** Parameter Value w/ Units
** Molecu 100.21
** Temperature 25° C
** Log Kow 4.5
** Water S 3.4 g/m3
** Vapor Pressure 6,133 Pa
** Melting Point -90.6° C
F020 258915
EOR
F002 483
F010 3.3.1
F004 3
F005 RS
F006 Using the Mackay Level I calculation, the following
** distribution is predicted for heptane:
**
** %Distri Compartment
** 99.91 Air
** <0.01 Water
** 0.08 Soil
** <0.01 Sediment
** <0.01 Suspended Sediment
** <0.01 Biota
F007 Using the Mackay Level I calculation, the following
** distribution is predicted for heptane:
**
** %Distri Compartment
** 99.91 Air
** <0.01 Water
** 0.08 Soil
** <0.01 Sediment
** <0.01 Suspended Sediment
** <0.01 Biota

F020 258916
EOR
F002 483
F010 3.3.1
F004 3
F005 TS
F006 CAS #142-82-5; heptane
F007 CAS #142-82-5; heptane
F020 258917
EOR
F002 483
F010 3.3.1
F004 4
F005 CL
F006 The majority of heptane is calculated to partition into the water phase,
* with smaller but significant amounts into air, soil, and sediment based
* on the modeling parameters used in this calculation. Heptane is
* considered to be a Type 1 chemi
F007 The majority of heptane is calculated to partition into the water phase,
* with smaller but significant amounts into air, soil, and sediment based
* on the modeling parameters used in this calculation. Heptane is
* considered to be a Type 1 chemical with potential to partition into all
* environmental compartments.
F020 258924
EOR
F002 483
F010 3.3.1
F004 4
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 cannot
* 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 258920
EOR
F002 483
F010 3.3.1
F004 4
F005 RE
F006 Mackay D (1998). Level III Fugacity-Based Environmental Equilibrium
* Partitioning Model, Version 2.1 (16-bit). Environmental Modelling Centre,
* Trent University, Ontario, Canada.
F007 Mackay D (1998). Level III Fugacity-Based Environmental Equilibrium
* Partitioning Model, Version 2.1 (16-bit). Environmental Modelling Centre,
* Trent University, Ontario, Canada.
F020 258926
EOR
F002 483
F010 3.3.1
F004 4
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 258925
EOR
F002 483
F010 3.3.1
F004 4
F005 RS
F006 Output:

**		Mass%	Emissions(kg/hr)
**	Air	26	1000
**	Water	48.5	1000
**	Soil	13.9	1000
**	Sedime	11.6	0

F007 Output:

**		Mass%	Emissions(kg/hr)
**	Air	26	1000
**	Water	48.5	1000
**	Soil	13.9	1000
**	Sedime	11.6	0

F020 258921
EOR
F002 483
F010 3.3.1
F004 4

F005 TC
F006 Physicochemical data used in the calculation:
**
** Parameter Value w/ Units
** Molecu 100.21
** Tempe 25° C
** Log Ko 4.5
** Water S 3.4 g/m3
** Vapor P 6,133 Pa
** Melting -90.6° C
**
** Reaction Half Lives in hours as predi
F007 Physicochemical data used in the calculation:
**
** Parameter Value w/ Units
** Molecu 100.21
** Tempe 25° C
** Log Ko 4.5
** Water S 3.4 g/m3
** Vapor P 6,133 Pa
** Melting -90.6° C
**
** Reaction Half Lives in hours as predicted using EPI SuiteTM:
**
** Air (gas 35.9
** Water (208
** Bulk Sc 416
** Bulk Se 1,870
**
** 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 258922
EOR
F002 483
F010 3.3.1
F004 4
F005 TS
F006 CAS #142-82-5; heptane
F007 CAS #142-82-5; heptane
F020 258923
EOR
F002 483
F010 3.5

F004 4
F005 CL
F006 Heptane is readily biodegradable.
F007 Heptane is readily biodegradable.
F020 258930
EOR
F002 483
F010 3.5
F004 4
F005 RE
F006 Haines J and Alexander M (1974). Microbial degradation of
* high-molecular-weight alkanes. Appl Microbiol 28:1084-1085.
F007 Haines J and Alexander M (1974). Microbial degradation of
* high-molecular-weight alkanes. Appl Microbiol 28:1084-1085.
F020 258932
EOR
F002 483
F010 3.5
F004 4
F005 RL
F006 A standard test method was used. The study was conducted prior to GLP.
F007 A standard test method was used. The study was conducted prior to GLP.
F020 258931
EOR
F002 483
F010 3.5
F004 4
F005 RS
F006 70% degradation was measured after 20 days incubation with an
* unacclimated inoculum.
** % Biodegradation of test substance after days:
** 2 days 0.28
** 5 days 0.63
** 10 days 0.7
** 20 days 0.7
F007 70% degradation was measured after 20 days incubation with an
* unacclimated inoculum.
** % Biodegradation of test substance after days:
** 2 days 0.28
** 5 days 0.63
** 10 days 0.7
** 20 days 0.7
F020 258927
EOR
F002 483
F010 3.5
F004 4
F005 TC
F006 American Public Health Association, Standard Methods for the Examination
* of Water and Waste Water, using 1.0 mg/l of test substance.
* Biodegradation was determined by measuring biological oxygen demand
* (BOD). Each 300 ml BOD bottle received

F007 American Public Health Association, Standard Methods for the Examination
* of Water and Waste Water, using 1.0 mg/l of test substance.
* Biodegradation was determined by measuring biological oxygen demand
* (BOD). Each 300 ml BOD bottle received 1.0 mg of heptane, 1.0 ml of a
* 1:10 suspension Hudson-Collamer silt loam soil in distilled water, and a
* mineral salts solution prepared as described in the test method. Bottles
* were incubated in the dark at 25C. The test substance was obtained from
* Aldrich Chemical Co.
F020 258928
EOR
F002 483
F010 3.5
F004 4
F005 TS
F006 CAS #142-82-5; heptane; 99% pure.
F007 CAS #142-82-5; heptane; 99% pure.
F020 258929
EOR
F002 483
F010 3.7
F004 2
F005 RE
F006 U.S. Environmental Protection Agency (U.S. EPA) (2000). EPI SuiteTM,
* Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.
F007 U.S. Environmental Protection Agency (U.S. EPA) (2000). EPI SuiteTM,
* Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.
F020 258936
EOR
F002 483
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 258935
EOR
F002 483
F010 3.7
F004 2
F005 RM
F006 A log bioconcentration factor (BCF) of 2.77 is calculated (BCF = 582).
* With respect to a log Kow = 4.50, which was used to calculate the BCF,
* heptane in the aquatic environment is expected to have a moderate
* potential to bioaccumulate.
F007 A log bioconcentration factor (BCF) of 2.77 is calculated (BCF = 582).
* With respect to a log Kow = 4.50, which was used to calculate the BCF,
* heptane in the aquatic environment is expected to have a moderate
* potential to bioaccumulate.
F020 258933
EOR

F002 483
F010 3.7
F004 2
F005 TS
F006 CAS #142-82-5; heptane
F007 CAS #142-82-5; heptane
F020 258934
EOR
F002 483
F010 4.1
F004 5
F005 ME
F006 ECOSAR version 0.99h, U.S. 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 h
F007 ECOSAR version 0.99h, U.S. 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 258937
EOR
F002 483
F010 4.1
F004 5
F005 RE
F006 ECOSAR v0.99h (2004) in EPI SuiteTM, U.S. EPA (2000). Estimation Program

* Interface Suite, v3.12. Syracuse Research Corporation, Syracuse, NY, USA.
F007 ECOSAR v0.99h (2004) in EPI SuiteTM, U.S. EPA (2000). Estimation Program
* Interface Suite, v3.12. Syracuse Research Corporation, Syracuse, NY, USA.
F020 258942
EOR
F002 483
F010 4.1
F004 5
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 258941
EOR
F002 483
F010 4.1
F004 5
F005 RS
F006 Calculated 96-hr LC50 for fish = 0.332 mg/L
F007 Calculated 96-hr LC50 for fish = 0.332 mg/L
F020 258938
EOR
F002 483
F010 4.1
F004 5
F005 TC
F006 Experimental water solubility = 3.4 mg/l @ 25°C (Yalkowsky and
* Dannenfelser, 1992), log Kow = 4.50 @ 25°C (Sangster, 1989), and melting
* point = -90.6°C (Lide et al., 1997-1998) were entered into the program.
** Class: Neutral organics
F007 Experimental water solubility = 3.4 mg/l @ 25°C (Yalkowsky and
* Dannenfelser, 1992), log Kow = 4.50 @ 25°C (Sangster, 1989), and melting
* point = -90.6°C (Lide et al., 1997-1998) were entered into the program.
** Class: Neutral organics
F020 258939
EOR
F002 483
F010 4.1
F004 5
F005 TS
F006 CAS #142-82-5; heptane
F007 CAS #142-82-5; heptane
F020 258940
EOR
F002 483
F010 4.2
F004 3
F005 ME
F006 Individual treatment concentrations were prepared by mixing the test
* substance in freshwater for 24 hours in a conical flask. The flask was
* almost completely filled with solution. After mixing, the treatment

* solutions were allowed to settle
F007 Individual treatment concentrations were prepared by mixing the test
* substance in freshwater for 24 hours in a conical flask. The flask was
* almost completely filled with solution. After mixing, the treatment
* solutions were allowed to settle for 24 hours. The aqueous solution was
* then drained through a stopcock at the base of the flask and tested. Test
* vessels were 250 ml conical flasks with 25 daphnids per flask. Two
* replicates of each treatment level and control were evaluated.
**
** Organisms supplied by testing lab; age = <24 hours old; parents age =
* approximately 21 days old.
F020 258944
EOR
F002 483
F010 4.2
F004 3
F005 ME
F006 Statistical method:
** Parametric model developed by Kooijman (Kooijman, S.A.L.M. 1981.
* Parametric analyses of mortality rate in bio-assays. Water Res.,
* 15:107-119.).
F007 Statistical method:
** Parametric model developed by Kooijman (Kooijman, S.A.L.M. 1981.
* Parametric analyses of mortality rate in bio-assays. Water Res.,
* 15:107-119.).
F020 258958
EOR
F002 483
F010 4.2
F004 3
F005 RE
F006 TNO, Division of Technology for Safety, Netherlands Organization for
* Applied Scientific Research (1986). Aquatic Toxicity of Compounds that
* may be Carried by Ships (MARPOL 1972, Annex II), Doc. # R 86/326a. TNO,
* The Netherlands.
F007 TNO, Division of Technology for Safety, Netherlands Organization for
* Applied Scientific Research (1986). Aquatic Toxicity of Compounds that
* may be Carried by Ships (MARPOL 1972, Annex II), Doc. # R 86/326a. TNO,
* The Netherlands.
F020 258949
EOR
F002 483
F010 4.2
F004 3
F005 RL
F006 This robust summary has a reliability rating of 2 because there is less
* raw data and information on the testing procedure than is desirable in
* order to rate this study for reliability at a level higher than 2. There
* is sufficient informatio
F007 This robust summary has a reliability rating of 2 because there is less
* raw data and information on the testing procedure than is desirable in
* order to rate this study for reliability at a level higher than 2. There

* is sufficient information in the report to suggest that the testing
* procedure generally followed an acceptable test guideline, OECD 202, and
* used acceptable methods to prepare exposure solutions.
F020 258948
EOR
F002 483
F010 4.2
F004 3
F005 RS
F006 48-hr EC50 for a daphnid = 0.423 mg/L
F007 48-hr EC50 for a daphnid = 0.423 mg/L
F020 258945
EOR
F002 483
F010 4.2
F004 3
F005 TC
F006 Dissolved oxygen was >50% saturation during the study. The pH was 7.5 to
* 8.3. Temperature was 20 Deg C.
**
** Analytical method used was Gas Chromatography with Flame Ionization
* Detection (GC-FID). Nominal treatment levels ranged from 0.32 to 10
F007 Dissolved oxygen was >50% saturation during the study. The pH was 7.5 to
* 8.3. Temperature was 20 Deg C.
**
** Analytical method used was Gas Chromatography with Flame Ionization
* Detection (GC-FID). Nominal treatment levels ranged from 0.32 to 10 mg/L.
* Only the following analytical data were reported:
**

**	Nomina	Initial Meas	48-hr Measured	
**	Conc. (	Conc. (mg/	Conc. (mg/L)	
**	0.32	0.04	Not Determined	
**	1	0.04	Not Determined	
**	3.2	0.5	Not Determined	
**	5.6	2.1		1.7
**	10	2.2	Not Determined	

F020 258946
EOR
F002 483
F010 4.2
F004 3
F005 TS
F006 CAS #142-82-5; heptane
F007 CAS #142-82-5; heptane
F020 258947
EOR
F002 483
F010 4.2
F004 4
F005 ME
F006 Individual treatment solutions were prepared by mixing the test substance
* in freshwater for 24 hours in conical flasks. The flask was almost

* completely filled with solution. After mixing, the treatment solutions
* were allowed to settle for 2
F007 Individual treatment solutions were prepared by mixing the test substance
* in freshwater for 24 hours in conical flasks. The flask was almost
* completely filled with solution. After mixing, the treatment solutions
* were allowed to settle for 24 hours. The aqueous solution was then
* drained through a stopcock at the base of the flask and tested. Test
* vessels were scintillation vials almost filled with approximately 20 ml
* of test solution and one organism per vial. Ten organisms were tested per
* treatment level. Organisms were transferred into fresh control and test
* solutions every 24 hours up to 96 hours.
**
** Organisms supplied by testing lab, grown in natural seawater with a
* salinity of 2.8%; length = 5 mm.
F020 258951
EOR
F002 483
F010 4.2
F004 4
F005 ME
F006 Statistical method:
** Parametric model developed by Kooijman (Kooijman, S.A.L.M. 1981.
* Parametric analyses of mortality rate in bio-assays. Water Res.,
* 15:107-119.).
F007 Statistical method:
** Parametric model developed by Kooijman (Kooijman, S.A.L.M. 1981.
* Parametric analyses of mortality rate in bio-assays. Water Res.,
* 15:107-119.).
F020 258957
EOR
F002 483
F010 4.2
F004 4
F005 RE
F006 TNO, Division of Technology for Safety, Netherlands Organization for
* Applied Scientific Research (1986). Aquatic Toxicity of Compounds that
* may be Carried by Ships (MARPOL 1972, Annex II), Doc. # R 86/326a. TNO,
* The Netherlands.
F007 TNO, Division of Technology for Safety, Netherlands Organization for
* Applied Scientific Research (1986). Aquatic Toxicity of Compounds that
* may be Carried by Ships (MARPOL 1972, Annex II), Doc. # R 86/326a. TNO,
* The Netherlands.
F020 258956
EOR
F002 483
F010 4.2
F004 4
F005 RL
F006 This robust summary has a reliability rating of 2 because there is less
* raw data and information on the testing procedure than is desirable in
* order to rate this study for reliability at a level higher than 2. There
* is sufficient informatio

F007 This robust summary has a reliability rating of 2 because there is less
* raw data and information on the testing procedure than is desirable in
* order to rate this study for reliability at a level higher than 2. There
* is sufficient information in the report to suggest that the testing
* procedure generally followed an acceptable test guideline and used
* acceptable methods to prepare exposure solutions.
F020 258955
EOR
F002 483
F010 4.2
F004 4
F005 RS
F006 96-hr LC50 for a gammarid = 0.2 mg/L
F007 96-hr LC50 for a gammarid = 0.2 mg/L
F020 258952
EOR
F002 483
F010 4.2
F004 4
F005 TC
F006 Dissolved oxygen was >50% saturation during the study. The pH was 7.5 to
* 8.3. Temperature was 15 Deg C. Natural seawater was used with a salinity
* of 2.8%
**
** Analytical method used was Gas Chromatography with Flame Ionization
* Detection (GC-FID
F007 Dissolved oxygen was >50% saturation during the study. The pH was 7.5 to
* 8.3. Temperature was 15 Deg C. Natural seawater was used with a salinity
* of 2.8%
**
** Analytical method used was Gas Chromatography with Flame Ionization
* Detection (GC-FID). Nominal treatment levels ranged from 0.32 to 10 mg/L.
* Test solutions were analyzed only upon test initiation.
**
** Only the following analytical data were reported:
**

** Nomina	Initial Measured
** Conc. (	Conc. (mg/L)
** 0.32	0.003
** 1	0.07
** 3.2	0.2
** 5.6	Not Determined
** 10	Not Determined

F020 258953
EOR
F002 483
F010 4.2
F004 4
F005 TS
F006 CAS #142-82-5; heptane
F007 CAS #142-82-5; heptane
F020 258954

EOR
F002 483
F010 4.2
F004 5
F005 ME
F006 Individual treatment solutions were prepared by mixing the test substance
* in freshwater for 24 hours in conical flasks. The flask was almost
* completely filled with solution. After mixing, the treatment solutions
* were allowed to settle for 2
F007 Individual treatment solutions were prepared by mixing the test substance
* in freshwater for 24 hours in conical flasks. The flask was almost
* completely filled with solution. After mixing, the treatment solutions
* were allowed to settle for 24 hours. The aqueous solution was then
* drained through a stopcock at the base of the flask and tested. Test
* vessels were scintillation vials almost filled with approximately 20 ml
* of test solution and one organism per vial. Ten organisms were tested per
* treatment level. Organisms were transferred into fresh control and test
* solutions every 24 hours up to 96 hours.
**
** Organisms supplied by testing lab, grown in natural seawater with a
* salinity of 2.8%; test organisms were approximately 4 weeks old, with
* lengths of approximately 6 mm.
F020 258959
EOR
F002 483
F010 4.2
F004 5
F005 ME
F006 Statistical method:
** Parametric model developed by Kooijman (Kooijman, S.A.L.M. 1981.
* Parametric analyses of mortality rate in bio-assays. Water Res.,
* 15:107-119.).
F007 Statistical method:
** Parametric model developed by Kooijman (Kooijman, S.A.L.M. 1981.
* Parametric analyses of mortality rate in bio-assays. Water Res.,
* 15:107-119.).
F020 258960
EOR
F002 483
F010 4.2
F004 5
F005 RE
F006 TNO, Division of Technology for Safety, Netherlands Organization for
* Applied Scientific Research (1986). Aquatic Toxicity of Compounds that
* may be Carried by Ships (MARPOL 1972, Annex II), Doc. # R 86/326a. TNO,
* The Netherlands.
F007 TNO, Division of Technology for Safety, Netherlands Organization for
* Applied Scientific Research (1986). Aquatic Toxicity of Compounds that
* may be Carried by Ships (MARPOL 1972, Annex II), Doc. # R 86/326a. TNO,
* The Netherlands.
F020 258965
EOR

F002 483
F010 4.2
F004 5
F005 RL
F006 This robust summary has a reliability rating of 2 because there is less
* raw data and information on the testing procedure than is desirable in
* order to rate this study for reliability at a level higher than 2. There
* is sufficient informatio
F007 This robust summary has a reliability rating of 2 because there is less
* raw data and information on the testing procedure than is desirable in
* order to rate this study for reliability at a level higher than 2. There
* is sufficient information in the report to suggest that the testing
* procedure generally followed an acceptable test guideline and used
* acceptable methods to prepare exposure solutions.
F020 258964
EOR
F002 483
F010 4.2
F004 5
F005 RS
F006 96-hr LC50 for a gammarid = 0.1 mg/L
F007 96-hr LC50 for a gammarid = 0.1 mg/L
F020 258961
EOR
F002 483
F010 4.2
F004 5
F005 TC
F006 Dissolved oxygen was >50% saturation during the study. The pH was 7.5 to
* 8.3. Temperature was 20 Deg C. Natural seawater was used with a salinity
* of 2.8%
**
** Analytical method used was Gas Chromatography with Flame Ionization
* Detection (GC-FID
F007 Dissolved oxygen was >50% saturation during the study. The pH was 7.5 to
* 8.3. Temperature was 20 Deg C. Natural seawater was used with a salinity
* of 2.8%
**
** Analytical method used was Gas Chromatography with Flame Ionization
* Detection (GC-FID). Nominal treatment levels ranged from 0.32 to 10 mg/L.
* Test solutions were analyzed only upon test initiation.
**
** Only the following analytical data were reported:
**
** Nomina Initial Measured
** Conc. (Conc. (mg/L)
** 0.32 0.003
** 1 0.07
** 3.2 0.2
** 5.6 Not Determined
** 10 Not Determined
F020 258962

EOR
F002 483
F010 4.2
F004 5
F005 TS
F006 CAS #142-82-5; heptane
F007 CAS #142-82-5; heptane
F020 258963
EOR
F002 483
F010 4.2
F004 6
F005 ME
F006 ECOSAR version 0.99h, U.S. 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 h
F007 ECOSAR version 0.99h, U.S. 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 258966
EOR
F002 483
F010 4.2
F004 6
F005 RE

F006 ECOSAR v0.99h (2004) in EPI SuiteTM, U.S. EPA (2000). Estimation Program
* Interface Suite, v3.12. Syracuse Research Corporation, Syracuse, NY, USA.
F007 ECOSAR v0.99h (2004) in EPI SuiteTM, U.S. EPA (2000). Estimation Program
* Interface Suite, v3.12. Syracuse Research Corporation, Syracuse, NY, USA.
F020 258971
EOR
F002 483
F010 4.2
F004 6
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 258970
EOR
F002 483
F010 4.2
F004 6
F005 RS
F006 Calculated 48-hr LC50 for a dahpnid = 0.423 mg/L
F007 Calculated 48-hr LC50 for a dahpnid = 0.423 mg/L
F020 258967
EOR
F002 483
F010 4.2
F004 6
F005 TC
F006 Experimental water solubility = 3.4 mg/l @ 25°C (Yalkowsky and
* Dannenfelser, 1992), log Kow = 4.50 @ 25°C (Sangster, 1989), and melting
* point = -90.6°C (Lide et al., 1997-1998) were entered into the program.
** Class: Neutral organics
F007 Experimental water solubility = 3.4 mg/l @ 25°C (Yalkowsky and
* Dannenfelser, 1992), log Kow = 4.50 @ 25°C (Sangster, 1989), and melting
* point = -90.6°C (Lide et al., 1997-1998) were entered into the program.
** Class: Neutral organics
F020 258968
EOR
F002 483
F010 4.2
F004 6
F005 TS
F006 CAS #142-82-5; heptane
F007 CAS #142-82-5; heptane
F020 258969
EOR
F002 483
F010 4.3
F004 2
F005 ME
F006 ECOSAR version 0.99h, U.S. 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 h
F007 ECOSAR version 0.99h, U.S. 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 258972
EOR
F002 483
F010 4.3
F004 2
F005 RE
F006 ECOSAR v0.99h (2004) in EPI SuiteTM, U.S. EPA (2000). Estimation Program
* Interface Suite, v3.12. Syracuse Research Corporation, Syracuse, NY, USA.
F007 ECOSAR v0.99h (2004) in EPI SuiteTM, U.S. EPA (2000). Estimation Program
* Interface Suite, v3.12. Syracuse Research Corporation, Syracuse, NY, USA.
F020 258977
EOR
F002 483
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 258976

EOR
F002 483
F010 4.3
F004 2
F005 RS
F006 Calculated 96-hr EC50 for a green alga = 0.305 mg/L
** Calculated 96-hr ChV for a green alga = 0.129 mg/L
F007 Calculated 96-hr EC50 for a green alga = 0.305 mg/L
** Calculated 96-hr ChV for a green alga = 0.129 mg/L
F020 258973
EOR
F002 483
F010 4.3
F004 2
F005 TC
F006 Experimental water solubility = 3.4 mg/l @ 25°C (Yalkowsky and
* Dannenfelser, 1992), log Kow = 4.50 @ 25°C (Sangster, 1989), and melting
* point = -90.6°C (Lide et al., 1997-1998) were entered into the program.
** Class: Neutral organics
F007 Experimental water solubility = 3.4 mg/l @ 25°C (Yalkowsky and
* Dannenfelser, 1992), log Kow = 4.50 @ 25°C (Sangster, 1989), and melting
* point = -90.6°C (Lide et al., 1997-1998) were entered into the program.
** Class: Neutral organics
F020 258974
EOR
F002 483
F010 4.3
F004 2
F005 TS
F006 CAS #142-82-5; heptane
F007 CAS #142-82-5; heptane
F020 258975
EOR
F002 483
F010 5.1.2
F004 1
F005 CL
F006 n-Heptane has a low order of toxicity by the inhalation route of exposure.
F007 n-Heptane has a low order of toxicity by the inhalation route of exposure.
F020 260310
EOR
F002 483
F010 5.1.2
F004 1
F005 RE
F006 HEDSET (1982). Acute Inhalation Toxicity Test, n-Heptane, Final Report.
F007 HEDSET (1982). Acute Inhalation Toxicity Test, n-Heptane, Final Report.
F020 260311
EOR
F002 483
F010 5.1.2
F004 1

F005 RM
F006 Animals were exposed to n-heptane vapor for 4 hours at a concentration of
* 29.29 mg/L (nominal) or 17937.5 ppm (mean analytical).
F007 Animals were exposed to n-heptane vapor for 4 hours at a concentration of
* 29.29 mg/L (nominal) or 17937.5 ppm (mean analytical).
F020 260308
EOR
F002 483
F010 5.1.2
F004 1
F005 RS
F006 There was no mortality during the course of the study. A slight
* reduction of mean male body weights was noted on day 2 post exposure but
* males recovered by day 4. All animals appeared normal throughout the
* study and at terminal necropsy w
F007 There was no mortality during the course of the study. A slight
* reduction of mean male body weights was noted on day 2 post exposure but
* males recovered by day 4. All animals appeared normal throughout the
* study and at terminal necropsy with the exception of one female observed
* with enlarged mandibular lymph nodes on the right side.
F020 260309
EOR
F002 483
F010 5.4
F004 1
F005 CL
F006 The effects observed are consistent with acute CNS depression and
* generally abated by the second week of study. Under the conditions of
* this study, the LOAEL for acute CNS depression is 2,970 ppm and the NOAEL
* for systemic toxicity is 2,97
F007 The effects observed are consistent with acute CNS depression and
* generally abated by the second week of study. Under the conditions of
* this study, the LOAEL for acute CNS depression is 2,970 ppm and the NOAEL
* for systemic toxicity is 2,970 ppm.
F020 260314
EOR
F002 483
F010 5.4
F004 1
F005 RE
F006 American Petroleum Institute (API) (1980). A 26 Week Inhalation Toxicity
* Study of Heptane in the Rat.
F007 American Petroleum Institute (API) (1980). A 26 Week Inhalation Toxicity
* Study of Heptane in the Rat.
F020 260315
EOR
F002 483
F010 5.4
F004 1
F005 RM
F006 Animals were exposed to 0, 398 or 2970 ppm n-heptane.
F007 Animals were exposed to 0, 398 or 2970 ppm n-heptane.

F020 260312
EOR
F002 483
F010 5.4
F004 1
F005 RM
F006 Type: 26-week inhalation toxicity study
** Number of animals: 15/sex/dose group
F007 Type: 26-week inhalation toxicity study
** Number of animals: 15/sex/dose group
F020 260316
EOR
F002 483
F010 5.4
F004 1
F005 RS
F006 There were no treatment-related deaths during the study. The only
* treatment-related observations were labored breathing or rapid breathing
* and slight prostration during the first week of study during exposure
* only, and anogenital fur and d
F007 There were no treatment-related deaths during the study. The only
* treatment-related observations were labored breathing or rapid breathing
* and slight prostration during the first week of study during exposure
* only, and anogenital fur and dry rales during weekly observations. The in
* chamber signs were generally more numerous and severe in the higher dose
* group and appeared to abate by the second week of the study.
**
** No treatment-related effects were observed for body weight, hematology or
* urinalysis. Serum alkaline phosphatase was significantly elevated in
* female high dose rats and slightly elevated in low dose females. All
* other clinical chemistry values appeared normal with the exception of one
* male high level rat whose serum glutamic pyruvic transaminase and serum
* alkaline phosphatase levels were markedly elevated when compared to all
* other male rats on test. Proteinuria, elevated specific gravity and
* ketones were observed but do not appear to be related to treatment.
F020 260313
EOR
F002 483
F010 5.4
F004 2
F005 CL
F006 Under the conditions of this test, inhalation of n-heptane at 1500 ppm
* did not induce neuropathy in rats.
F007 Under the conditions of this test, inhalation of n-heptane at 1500 ppm
* did not induce neuropathy in rats.
F020 260320
EOR
F002 483
F010 5.4
F004 2
F005 RE
F006 Frontali N, Amantini MC, Spagnolo A, Guarcini AM, Saltari MC, Brugnone F

* and Perbellini L (1981). Experimental Neurotoxicity and Urinary
* Metabolites of the C5-C7 Aliphatic Hydrocarbons Used as Glue Solvents in
* Shoe Manufacture. Clin Toxic
F007 Frontali N, Amantini MC, Spagnolo A, Guarcini AM, Saltari MC, Brugnone F
* and Perbellini L (1981). Experimental Neurotoxicity and Urinary
* Metabolites of the C5-C7 Aliphatic Hydrocarbons Used as Glue Solvents in
* Shoe Manufacture. Clin Toxicol 18(12):1357-1367.
F020 260321
EOR
F002 483
F010 5.4
F004 2
F005 RM
F006 Only males and one dose group were used. The primary objective of this
* study was to assess the appearance of polyneuropathy and urinary
* metabolites in rats following exposure to analytical grade solvents
* frequently used in Italian shoe fac
F007 Only males and one dose group were used. The primary objective of this
* study was to assess the appearance of polyneuropathy and urinary
* metabolites in rats following exposure to analytical grade solvents
* frequently used in Italian shoe factories. Nerve tissue was examined
* microscopically.
**
** Body weights were analyzed by a two-way analysis of variance and
* Student's t test for the comparison of two slopes.
F020 260317
EOR
F002 483
F010 5.4
F004 2
F005 RM
F006 Type: 30-week inhalation neurotoxicity study
** Number of animals: 6-9 males/dose group
F007 Type: 30-week inhalation neurotoxicity study
** Number of animals: 6-9 males/dose group
F020 260318
EOR
F002 483
F010 5.4
F004 2
F005 RS
F006 None of the animals developed signs of neuropathy. There were no
* differences in weight gain of rats (30 weeks) compared to controls.
* Differences between mean values for hindlimb spreads observed in treated
* animals and controls were not st
F007 None of the animals developed signs of neuropathy. There were no
* differences in weight gain of rats (30 weeks) compared to controls.
* Differences between mean values for hindlimb spreads observed in treated
* animals and controls were not statistically significant. However,
* authors note that in their hands, the test employed turned out to be
* scarcely effective due to high individual variability. No histological
* signs of giant axonal degeneration were noted in rats treated at 1500 ppm

* (30 weeks).
F020 260319
EOR
F002 483
F010 5.5
F004 1
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 260325
EOR
F002 483
F010 5.5
F004 1
F005 RE
F006 Brooks TM, Meyer AL and Hutson, DH (1982). The genetic toxicology of some
* hydrocarbon and oxygenated solvents. Mutagenesis 3:227-232.
F007 Brooks TM, Meyer AL and Hutson, DH (1982). The genetic toxicology of some
* hydrocarbon and oxygenated solvents. Mutagenesis 3:227-232.
F020 260326
EOR
F002 483
F010 5.5
F004 1
F005 RM
F006 GLP: Quality assurance statement
F007 GLP: Quality assurance statement
F020 260323
EOR
F002 483
F010 5.5
F004 1
F005 RM
F006 Strains tested: Salmonella typhimurium tester strains TA98, TA100,
* TA1535, TA1537, TA1538; Escherichia coli strains WP2, WP uvr A
**
** Test substance concentrations: 3.91, 7.81, 15.6, 31.3, 62.5, 125, 250
* mg/ml
**
** Metabolic activation: With
F007 Strains tested: Salmonella typhimurium tester strains TA98, TA100,
* TA1535, TA1537, TA1538; Escherichia coli strains WP2, WP uvr A
**
** Test substance concentrations: 3.91, 7.81, 15.6, 31.3, 62.5, 125, 250
* mg/ml
**
** Metabolic activation: With and without (S9 fraction mix of livers from
* Aroclor 1254 pretreated rats)
**
** Vehicle: Tween 80/ethanol
**
** Positive Controls: benzo[a]pyrene, 4-nitroquinoline-N-oxide, sodium

* azide, neutral red, potassium dichromate.
**
** Cytotoxicity study: A toxicity screening test conducted prior to the
* full assay indicated cytotoxicity at 500 mg/ml with and without metabolic
* activation.
**
** The cultures were incubated at 37°C for 48-72 hours in a sealed container
* before the revertant colonies were counted. Pre-incubation method was
* used to limit evaporation of test material.
F020 260322
EOR
F002 483
F010 5.5
F004 1
F005 RS
F006 The addition of heptane at amounts up to 250 mg per ml to cultures of
* Escherichia coli WP2 and WP2 uvr A, Salmonella typhimurium TA 1535, TA
* 1537, TA 1538, TA 98, and TA 100 did not lead to an increase in the
* reverse gene mutation frequenc
F007 The addition of heptane at amounts up to 250 mg per ml to cultures of
* Escherichia coli WP2 and WP2 uvr A, Salmonella typhimurium TA 1535, TA
* 1537, TA 1538, TA 98, and TA 100 did not lead to an increase in the
* reverse gene mutation frequency in any of these strains, either in the
* presence or in the absence of rat liver S9 fraction. In one assay with
* Escherichia coli WP2 in the presence of S9 fraction a greater than 2.5
* fold increase over control values was seen at 15.6 and 31.3 mg per ml.
* This increase was not dose-related nor repeated in replicate assays and
* was therefore not considered to be a compound-related effect.
F020 260324
EOR
F002 483
F010 5.5
F004 2
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 260332
EOR
F002 483
F010 5.5
F004 2
F005 RE
F006 Brooks TM, Meyer AL and Hutson, DH (1982). The genetic toxicology of some
* hydrocarbon and oxygenated solvents. Mutagenesis 3:227-232.
F007 Brooks TM, Meyer AL and Hutson, DH (1982). The genetic toxicology of some
* hydrocarbon and oxygenated solvents. Mutagenesis 3:227-232.
F020 260327
EOR
F002 483
F010 5.5
F004 2
F005 RM

F006 GLP: Quality assurance statement
F007 GLP: Quality assurance statement
F020 260330
EOR
F002 483
F010 5.5
F004 2
F005 RM
F006 Strains tested: Saccharomyces cerevisiae JD1
**
** Test substance concentrations: 0.01, 0.1, 0.5, 1.0, 5.0 mg/ml
**
** Metabolic activation: With and without (S9 fraction mix of livers from
*   Aroclor 1254 pretreated rats)
**
** Vehicle: Tween 80/ethanol
F007 Strains tested: Saccharomyces cerevisiae JD1
**
** Test substance concentrations: 0.01, 0.1, 0.5, 1.0, 5.0 mg/ml
**
** Metabolic activation: With and without (S9 fraction mix of livers from
*   Aroclor 1254 pretreated rats)
**
** Vehicle: Tween 80/ethanol
**
** Positive Controls: 4-nitroquinoline-N-oxide, cyclophosphamide
**
** After 18-hour incubation at 30°C the cultures were placed onto the
*   appropriate culture media for the selection of prototrophic colonies.
*   After three days incubation at 30°C the numbers of prototrophic colonies
*   were counted.
F020 260329
EOR
F002 483
F010 5.5
F004 2
F005 RS
F006 Exposure of Saccharomyces cerevisiae JD1 to heptane at concentrations up
*   to 5.0 mg/ml did not result in a consistent increase in the rate of
*   mitotic gene conversion, either in the presence or in the absence of rat
*   liver S9 fraction.
F007 Exposure of Saccharomyces cerevisiae JD1 to heptane at concentrations up
*   to 5.0 mg/ml did not result in a consistent increase in the rate of
*   mitotic gene conversion, either in the presence or in the absence of rat
*   liver S9 fraction.
F020 260331
EOR
F002 483
F010 5.5
F004 3
F005 CL
F006 Under the conditions of this study, the test material was not clastogenc.

F007 Under the conditions of this study, the test material was not clastogenc.
F020 260336
EOR
F002 483
F010 5.5
F004 3
F005 RE
F006 Brooks TM, Meyer AL and Hutson, DH (1982). The genetic toxicology of some
* hydrocarbon and oxygenated solvents. Mutagenesis 3:227-232.
F007 Brooks TM, Meyer AL and Hutson, DH (1982). The genetic toxicology of some
* hydrocarbon and oxygenated solvents. Mutagenesis 3:227-232.
F020 260328
EOR
F002 483
F010 5.5
F004 3
F005 RM
F006 GLP: Quality assurance statement
F007 GLP: Quality assurance statement
F020 260333
EOR
F002 483
F010 5.5
F004 3
F005 RM
F006 Vehicle: Tween 80/ethanol
**
** Positive Controls: 7,12-Dimethylbenzanthracene (DMBA)
**
** Cultured rat liver cells were grown and treated on glass microscopic
* slides contained in 100-ml volume glass Leighton tubes. After 22-hour
* exposure to tes
F007 Vehicle: Tween 80/ethanol
**
** Positive Controls: 7,12-Dimethylbenzanthracene (DMBA)
**
** Cultured rat liver cells were grown and treated on glass microscopic
* slides contained in 100-ml volume glass Leighton tubes. After 22-hour
* exposure to test compound or vehicle, colcemid was added to each culture.
* After further 2 hours, the slides were removed, subjected to hypotonic
* treatment followed by fixation (methanol:acetic acid, 3:1) and stained
* with Giemsa. The preparations were randomly coded and 100 cells from
* each culture were analyzed microscopically.
F020 260334
EOR
F002 483
F010 5.5
F004 3
F005 RS
F006 In one culture exposed to 10 mg/ml of heptane a total of 7 chromatid gaps
* were seen; this increased the frequency to 0.024 gaps per cell which,
* although greater than the vehicle control frequency, was not accompanied

* by an increase in any o
F007 In one culture exposed to 10 mg/ml of heptane a total of 7 chromatid gaps
* were seen; this increased the frequency to 0.024 gaps per cell which,
* although greater than the vehicle control frequency, was not accompanied
* by an increase in any other type of aberration and is not considered to
* be a compound-related effect. Thus there was no significant or
* dose-related increase of chromosome damage in any of the culture exposed
* to heptane.
** Cultures exposed to the positive control material, DMBA, showed a marked
* increase in the frequency of chromosome damage.
F020 260335
EOB
C
X