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JuanB Perez/DC/USEPA/US
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To NCIC HPV@EPA
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Subject

----- Forwarded by JuanB Perez/DC/USEPA/US on 06/12/2007 02:29 PM -----

murrayj7210@comcast.net
06/11/2007 01:08 PM

To Rtk Chem@EPA, NCIC OPPT@EPA
cc
Subject

HPV Program

Attached please find the Para Toluenesulfonic Acid Coalition's submittal of a the submittal letter and a complete dossier for para-Toluenesulfonic Acid (p-TSA) (CAS No. 104-15-4.

PLEASE FORWARD A RESPONSE OF RECEIPT OF THESE DOCUMENT TO THE P-TSA COALITION.

If there are any questions, please contact me directly. Thank you for your attention to the above.

Sincerely

John F. (Jack) Murray, CAE
para-Toluenesulfonic Acid Coalition
Telephone 301-651-5051
E-Mail murrayj7210@comcast.net

p-TSA submittal to EPA's orphan HPV program..doc

pTSA HPV Submittal to EPA Final.doc

Please verify receipt of this submission by return e-mail.

201-16597

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June 11, 2007

Dr. Oscar Hernandez
Director, Risk Assessment Division
Environmental Protection Agency
7403M
USEPA Headquarters
Ariel Rios Building
1200 Pennsylvania Avenue, N. W.
Washington, DC 20460

Dear Dr. Hernandez:

Re: SOCMA Para Toluenesulfonic Acid Coalition's (p-TSA) submission of a complete dossier for the orphan chemical HPV Challenge program:

The SOCMA Paratoluenesulfonic Acid Coalition (p-TSA) submits the enclosed dossier on p-Toluenesulfonic acid (CAS# 104-15-4).

If you have any questions, please contact me directly.

Sincerely;

John F. (Jack) Murray, CAE
Executive Director
Phone: 301-651-5051
E-mail: murrayj7210@comcast.net

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2007 JUN 13 AM 7:30

201-16597A

HPV Assessment Report
on
p-Toluenesulphonic acid
CAS No. 104-15-4

June, 2007

Submitted on behalf of the p-Toluenesulphonic Acid Coalition.
1850 M Street, NW, Suite 700, Washington DC 20036

Prepared by NOTOX Safety and Environmental Research B.V.
for submission under the US-HPV Challenge Program

Contents

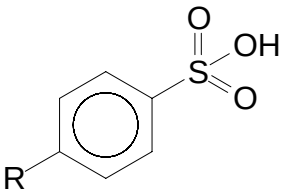
1. Introduction

Capital Resin Corporation, Dynachem, Inc. and Rütgers Organics Corporation formed a consortium known as the Aromatics Sulfonic Acids Association (ASAA) to participate in the United States High Production Volume (HPV) Chemical Challenge Program. This consortium supported benzenesulphonic acid, (CASRN 98-11-3) and hydroxybenzenesulphonic acid, (CASRN 1333-39-7). A new consortium formed by Capital Resins Corporation, DynaChem, Incorporated, InterTrade Holdings, Incorporated, Nease Corporation, Sloss Industries Corporation and Stepan Company has taken the initiative to support the orphan chemical p-toluenesulphonic acid (CASRN 104-15-4). The substance is also known as 4-methylbenzenesulphonic acid. Aromatic sulfonic acids, such as para toluene sulfonic acids (p-TSA) are made by sulfonating aromatic compounds with sulfonic acid, $SO_{3,}$ or Oleum. pTSA is comparable in strength to mineral acids such as sulphuric acid, but are especially suitable for organic reactions where an inorganic, mineral acid could cause charring, oxidation, or an unwanted chemical reaction. It is most useful as an esterification/condensation/acetylation catalyst and as an acid catalyst for resins in foundry cores. Other uses include: curing agent for Amino/phenolic/acrylic resins, descaling agent (industrial metal cleaners), electroplating bath additive, plastics, coatings, dyes, pharmaceutical intermediates, hydrotrope, coupling agent and as a wetting agent. Also applicable for use in food packaging adhesives. The substance is classified as a high production volume (HPV) chemical according to the criterium established by the US-EPA, (i.e., > 1,000,000 pounds manufactured or imported into the USA annually). The consortium has agreed to provide all internal documents related to the requirements of the Challenge Program and/or initiate scientifically justified studies for this chemical substance as required to meet the needs of the HPV Chemical Challenge Program.

Under agreement with the consortium, NOTOX Safety and Environmental Research B.V. has conducted an evaluation and assessment of the available data on p-toluenesulphonic acid (CASRN 104-15-4). For health and environmental assessment information, data available from the HPV assessment on benzenesulphonic acid (with p-toluenesulphonic acid as surrogate) were used. The rationale for the similarity between these two substances and to use now benzenesulphonic acid as a surrogate for p-toluenesulphonic acid is described in chapter 2. The studies retrieved on p-toluenesulphonic acid and benzenesulphonic acid meeting the SIDS data requirements are summarised in chapter 3. A SIDS data matrix was constructed and recommendations for the draft testing scheme were formulated (data availability analysis; chapter 4). Robust summaries are presented in appendices as IUCLID data sets.

2. Rationale for the surrogate benzenesulphonic acid

For p-toluenesulphonic acid (CASRN 104-15-4), the closely related substance benzenesulphonic acid (CASRN 98-11-3) can be used as a surrogate in view of the chemical similarity between the two compounds (see Figure 1). The extra methyl group para to the sulphonic acid group in p-toluenesulphonic acid has a weakly activating effect on the benzene ring, which makes it slightly more prone to electrophilic aromatic substitution.
Acidity of the sulphonic acid group is influenced by two factors:
1. The methyl group exerts an electron donating effect, which makes the negative charge on the resulting sulphonate ion after deprotonation slightly less stable.
2. The resonance effect still stabilises the negative charge on the sulphonate ion by dividing the charge on the oxygen atoms.
As a result, the acidity of the sulphonic acid group is not expected to change significantly compared to benzenesulphonic acid. Calculation of the pKa confirms this expectation: –2.58 for p-toluenesulphonic acid and –2.8 for benzenesulphonic acid.
Thus the reactivity of p-toluenesulphonic acid and benzenesulphonic acid is very similar and aquatic toxicity data from benzenesulphonic acid can be used for p-toluenesulphonic acid.



CASRN
98-11-3 R=H
104-15-4 R=CH_3

Figure 1. Structure of benzenesulphonic acid (CASRN 98-11-3) and p-toluenesulphonic acid (CASRN 104-15-4).

3. Evaluation of SIDS endpoints

In this chapter an evaluation of data available on SIDS endpoints is given.

p-Toluenesulphonic acid and benzenesulphonic acid are strong acids (comparable to sulphuric acid). In watery environments they are almost completely ionised even at low pH. The typical commercial preparations used as catalysts are 65-70% solutions in water.

3.1. Physico-chemical endpoints

For p-toluenesulphonic acid data on melting point, boiling point, vapor pressure (calculated), partition coefficient (calculated), water solubility and dissociation constant (calculated) are available. The physico-chemical properties of benzenesulphonic acid are very similar to those of p-toluenesulphonic acid (see Table below). The calculated values for vapor pressure for both substances are all very low as expected. The calculated values for the partition coefficient indicate that both sulphonic acids dissolve to a much larger extent in water than in octanol as expected from the structural formulas and the dissociation constants indicate that these substances are predominantly ionised in water even at low pH. The measured water solubility of p-toluenesulphonic acid seems to be lower than for benzenesulphonic acid (calculated). A lower solubility for p-toluenesulphonic acid may be expected based on the presence of the extra methyl group that renders p-toluenesulphonic acid more hydrophobic, but both sulphonic acids are considered to be highly soluble (>100 grams/liter) in water.

	p-Toluenesulphonic acid CAS 104-15-4				**Benzenesulphonic acid CAS 98-11-3**			
	Value	**Comment**	**Kl.**	**Ref**	**Value**	**Comment**	**Kl.**	**Ref**
Melting point (°C)	106-107	anhydrous	2	1,2	50-51	anhydrous	4	1,2
Boiling point (°C)	140	measured at 26.7 hPa	2	1	171-172	measured at 0.13 hPa[1]	2	17
	332	calculated at 1013 hPa	2	3	319	calculated at 1013 hPa	2	3
Vapor pressure (hPa)	3.9E-06	calculated at 25°C	2	3	2.28E-05	calculated at 25°C	2	3
					2.2E-09	Watson (at 20°C)	1	19
Partition coefficient (log K_{ow})	-0.62	calculated	2	3	-1.17	calculated	2	3
Water solubility (g/L at 25 °C)	670	measured	2	2	689.5	calculated	2	3
	202.3	calculated	2	3				
	620	exp. database	2	3				
Dissociation constant (pKa)	-2.58	calculated	2	4	0.7 at 25 °C		2	2
					-2.80	calculated	2	4

[1] is estimated to be equal to 403 °C at atmospheric pressure.
Kl. = Klimisch criteria
Ref = Reference number

Conclusion: For the physico-chemical endpoints all relevant endpoints are sufficiently investigated.

3.2. Environmental fate

The half-life for reaction with hydroxyl radicals in the atmosphere was estimated to be similar for both substances. No hydrolysable groups are present in p-toluenesulphonic acid or benzenesulphonic acid. Distribution in the environment was calculated at Mackay Level III. If the sulphonic acids are released to the environment it will be to the water compartment (see table below). Including this in the program, both substances were found to stay in the water compartment.
No standard OECD301B or 301D microbial biodegradation studies are available on p-toluene-sulphonic acid. p-Toluenesulphonic acid is reported to be biodegradable for more than 90% in 5 days in two aerobic tests. It cannot be concluded that p-toluenesulphonic acid is readily biodegradable because no standard, detailed described tests are available. In a study with adapted sludge both substances were degraded at the same rate (98.7% and 98.5% based on COD for p-toluene- and benzenesulphonic acid, respectively); the time elapsed is, however, not given. Another test with p-toluenesulphonic acid using adapted sludge resulted in 90% degradation after 24 hours. Based on the scientific literature it can be concluded by weight of the evidence that p-toluenesulphonic acid is biodegradable, but not whether the substance is readily biodegradable.

Conclusion: For all relevant endpoints on environmental fate, adequate data are available. The data available on biodegradation of both substances indicate that biodegradation is a pathway for removal from the environment. No further testing is recommended.

	p-Toluenesulphonic acid CAS 104-15-4				**Benzenesulphonic acid CAS 98-11-3**			
	Value	**Comment**	**Kl.**	**Ref**	**Value**	**Comment**	**Kl.**	**Ref**
Photodegradation (t1/2)	7.8 days	calculated	2	3	19.2 days	calculated	2	3
Hydrolysis (t1/2)	no				no			
Distribution in water/air/soil/sediment	99.8/0.0/0.0/0.17%	calculated (emission to water only)	2	3	99.8/0.0/0.0/0.17%	calculated (emission to water only)	2	3
Biodegradability	degradable		4	5,9,13,14	degradable		4	13

Kl. = Klimisch criteria
Ref = Reference number

3.3. Ecotoxicity

For p-toluenesulphonic acid, an adequate acute fish study was reviewed that shows the absence of toxicity to this substance. The experimental result available for a daphnia acute study (>1625 mg/L) confirms this. The acute daphnia EC50 for benzenesulphonic acid (>100 mg/L; highest concentration tested) also shows that no toxicity to daphnia is to be expected for this surrogate. For benzenesulphonic acid an algal test according to OECD 201 indicates slight toxicity to these organisms (EC_{50} = 73 mg/L), probably due to the acidity of the test substance. Since both substances have similar (calculated) physicochemical properties, and the values for acute daphnia toxicity coincide, the experimental value for algal toxicity for p-toluenesulphonic acid is expected to be at a similar slight-toxic level as the value of benzenesulphonic acid and the value can be read-across to p-toluenesulphonic acid.

Conclusion: Adequate data for all ecotoxicity endpoints are available.

	p-Toluenesulphonic acid CAS 98-11-3				Benzenesulphonic acid CAS 104-15-4			
	Value	**Comment**	**KL.**	**Ref**	**Value**	**Comment**	**Kl.**	**Ref**
Acute fish (96-h LC50, mg/L)	>325		2	8	-			
Acute invertebrates (48-h EC50, mg/L)	>1625	exp. time not indicated	4	9	>100	OECD202	1	20
Algal inhibition (96-h EC50, mg/L)	read-across				73	OECD201	1	21

Kl. = Klimisch criteria
Ref = Reference number

3.4. Mammalian toxicity

Sulphonic acids are very acidic (comparable to sulphuric acid) and are expected to show local effects in the gastrointestinal tract. The dissociation constant is low and, therefore, absorption is expected to be low in the gastrointestinal tract. Dermal absorption is expected to be low, because the partition coefficient is low.
p-Toluenesulphonic acid is classified as irritant to skin, eyes and inhalatory system (www.inchem.org). In a skin irritation study p-toluenesulphonic acid caused burns. This is due to the acidic nature of the test substance.
Although benzene-sulphonic acid is not used as a surrogate for mammalian toxicity, available data is presented in the table below to show the equivalence in properties of the two substances.

3.4.1. Acute toxicity

An acute oral test according to OECD 401 was available for p-toluenesulphonic acid resulting in an LD_{50} value of 1410 mg/kg bw for rat. The main effect was injury to the gastrointestinal tract.

3.4.2. Genetic toxicity

For p-toluenesulphonic acid an adequate Ames test and chromosomal aberration test are available, both with a negative result. Therefore this endpoint has been sufficiently investigated.

3.4.3. Repeated dose toxicity

A 28-day study performed according to OECD 407 and summarised in the ECB-IUCLID is available for p-toluenesulphonic acid to satisfy this endpoint. Although the information given is limited, the NOAEL for systemic effects was reported to be > 500 mg/kg (the highest concentration tested).

3.4.4. Repro/developmental toxicity

No data are available on this endpoint. However, taking into consideration the corrosive nature of the aromatic sulphonic acids discussed above, conducting a repeated dose study would cause unnecessary harm to laboratory animals. Moreover, because of their high polarity and high water solubility, the substances would be expected to be absorbed into systemic circulation to a minimal extent. For these reasons, testing of repro/developmental toxicity will not be done.

Conclusion mammalian toxicity: Acute toxicity has been sufficiently investigated. For genetic toxicity adequate data are available. For repeated dose toxicity a summary of a 28-day study is available. Repro/developmental toxicity will not be tested because of the corrosive nature of the substance.

	p-Toluenesulphonic acid CAS 104-15-4				**Benzenesulphonic acid CAS 98-11-3**			
	Value	**Comment**	**KL.**	**Ref**	**Value**	**Comment**	**Kl.**	**Ref**
Acute toxicity								
Acute oral (LD50, mg/kg bw)	1410	rat	1	10	1100	rat	2	6
Acute dermal (LD50, mg/kg bw)	-				-			
Acute inhalation (LC50, mg/m^3)	-				-			
Genetic toxicity								
in vitro gene mutation (Ames test)	negative	no E.coli	1	11	negative	no E.coli	2	7
Chromosomal aberration	negative		1	12	-			
Repeated dose	>500 mg/kg bw	NOAEL; highest dose tested	4	18	-			
Repro/developmental toxicity	-				-			

Kl. = Klimisch criteria
Ref = Reference number

3.5. SIDS Data matrix

Summary of the available data for all SIDS endpoints.

	p-Toluenesulphonic acid CAS 104-15-4				**Benzenesulphonic acid CAS 98-11-3**			
	Value	**Comment**	**KL.**	**Ref**	**Value**	**Comment**	**Kl.**	**Ref**
Physico-chemical								
Melting point (°C)	106-107	anhydrous	2	1,2	50-51	anhydrous	4	1,2
Boiling point (°C)	140	measured at 26.7 hPa	2	1	171-172	measured at 0.13 hPa[1]	2	17
	332	calculated at 1013 hPa	2	3	319	calculated at 1013 hPa	2	3
Vapor pressure (hPa)	3.9E-06	calculated at 25°C	2	3	2.28E-05	calculated at 25°C	2	3
					2.2E-09	Watson (at 20°C)	1	19

	p-Toluenesulphonic acid CAS 104-15-4				Benzenesulphonic acid CAS 98-11-3			
	Value	**Comment**	**KL.**	**Ref**	**Value**	**Comment**	**Kl.**	**Ref**
Partition coefficient (log K_{ow})	-0.62	calculated	2	3	-1.17	calculated	2	3
Water solubility (g/L at 25 °C)	670	measured	2	2	689.5	calculated	2	3
	202.3	calculated	2	3				
	620	exp. database	2	3				
Dissociation constant (pKa)	-2.58	calculated	2	4	0.7 at 25 °C		2	2
					-2.80	calculated	2	4
Environmental fate								
Photodegradation (t1/2)	7.8 days	calculated	2	3	19.2 days	calculated	2	3
Hydrolysis (t1/2)	no				no			
Distribution in water/air/soil/sediment	99.8/0.0/0.0/0.17%	calculated (emission to water only)	2	3	99.8/0.0/0.0/0.17%	calculated (emission to water only)	2	3
Biodegradability	degradable		4	5,9, 13,14	degradable		4	13
Ecotoxicity								
Acute fish (96-h LC50, mg/L)	>325		2	9	-			
Acute invertebrates (48-h EC50, mg/L)	>1625	exp. time not indicated	4	9	>100	OECD202	1	20
Algal inhibition (96-h EC50, mg/L)	read-across				73	OECD201	1	21
Mammalian toxicity								
Acute toxicity								
Acute oral (LD50, mg/kg bw)	1410	rat	1	10	1100	rat	2	6
Acute dermal (LD50, mg/kg bw)	-				-			
Acute inhalation (LC50, mg/m^3)	-				-			
Genetic toxicity								
in vitro gene mutation (Ames test)	negative	no E.coli	1	11	negative	no E.coli	2	7
Chromosomal aberration	negative		1	12	-			
Repeated dose	>500 mg/kg bw	NOAEL; highest dose tested	4	18	-			
Repro/developmental toxicity	-				-			

Kl. = Klimisch criteria, Ref = Reference number

4. Data availability and testing proposal

The availability of data is depicted in the following table.

	p-Toluenesulphonic acid CAS 104-15-4
Physico-chemical	
Melting point	+
Boiling point	+
Vapor Pressure	+
Partition Coefficient	+
Water Solubility	+
Environmental Fate	
Photodegradation	+
Hydrolysis	+
Distribution into compartments	+
Biodegradability	+
Ecotoxicity	
96-h LC50 Fish	+
48-h EC50 Daphnia	+
72-h EC50 Algal Inhibition	+ (read-across)
Mammalian toxicity	
Acute	+
Repeated dose	+
Genetic	+
Reproduction/developmental	no test

+ = data available
read-across = using data from surrogate benzenesulphonic acid

Adequate physicochemical, environmental and ecotoxicity data are available. Genetic toxicity has been sufficiently investigated. Based on the corrosivity of the test substance and the presence of a repeated dose study for p-toluenesulphonic acid, no testing will be done for reproduction/-developmental toxicity.

5. References

(1) SAX's Dangerous Properties of Industrial Materials, (Ed. R.J. Lewis Sr., 9th Ed., Van Nostrand Reinhold, NY, 1996.

(2) Merck Index, CD-rom 2000.

(3) EPISuite v.3.10, April 2001.

(4) Pallas 2.1, 1994/95.

(5) Matsui, S.; Y. Okawa & R. Ota, Experience of 16 years' operation and maintenance of the Fukashiba industrial wastewater treatment plant of the Kashima petrochemical complex - II. Biodegradability of 37 organic substances and 28 process wastewaters, Water Sci. Technol. 20: 201-210, 1988.

(6) Smythe, HF; Carpenter, CP; Weil, CS; Pozzani, UC; Striegel, JA; American Ind. Hygiene Association Journal 23: 95-107, 1962.

(7) Zeiger, E; Anderson, B; Haworth, S; Lawlor, T; Mortelmans, K; Speck, W; Salmonella mutagenicity tests: III. Results from the testing of 255 chemicals, Environmental Mutagenesis 9 (Suppl.9): 1-110, 1988.

(8) Hoechst AG, Akute Toxizitaet von p-Toluolsulfonsaeure Loesung 65%ig an Goldorfen, Bericht 197/81, 1981.

(9) Hoechst AG, internal report, Bericht W82-360 (23.3.1983).

(10) Hoechst AG, p-Toluolsulfonsaeure: Pruefung der akuten oralen Toxizitaet an der Wistar-Ratte, Bericht 88.1563, 1988.

(11) Hoechst AG, EXT 8804 p-Toluenesulfonic acid: Reverse mutation assay in vitro Ames test, Bericht 88.0892, 1988.

(12) Hoechst AG, p-Toluolsulfonsaeure: Chromosome aberrations in vitro in V79 chinese hamster cells, Report No. 88.1940, 1988.

(13) Pitter, P., Determination of biological degradability of organic substances, Water Res. 10: 231-235, 1976.

(14) Hoechst AG, internal report (31.8.1978).

(15) Matsui, S.; Y. Okawa & R. Ota, Experience of 16 years' operation and maintenance of the Fukashiba industrial wastewater treatment plant of the Kashima petrochemical complex - II. Biodegradability of 37 organic substances and 28 process wastewaters, Water Sci. Technol. 20: 201-210, 1988.

(16) Hoechst AG, internal report (07.12.1972).

(17) Lindner, O., Ullmann's Encyclopedia of Industrial Chemistry, Ed. W. Gerhartz, 5th Ed., VCH Verlag, A3, 1985, p.515, 517-518.

(18) Hoechst AG (1990): Internal report No. 90.0037 in IUCLID Dataset Toluene-4-sulphonic acid (CAS No. 104-15-4) on IUCLID CD-ROM, 2000.

(19) NOTOX BV, Calculation of the vapour pressure of benzenesulphonic acid, Project 408847, 2004.

(20) NOTOX BV, Acute toxicity study in Daphnia magna with benzenesulfonic acid (static), Project 418725, 2005.

(21) NOTOX BV, Fresh water algal growth inhibition test with benzenesulfonic acid, Project 418736, 2005.

Appendix 1

I U C L I D

Data Set

Existing Chemical	:	ID: 104-15-4
CAS No.	:	104-15-4
EINECS Name	:	toluene-4-sulphonic acid
EC No.	:	203-180-0
TSCA Name	:	Benzenesulfonic acid, 4-methyl-
Molecular Formula	:	C7H8O3S

Producer related part

Company	:	Notox
Creation date	:	25.06.2003

Substance related part

Company	:	Notox
Creation date	:	25.06.2003
Status	:	
Memo	:	
Printing date	:	03.07.2006
Revision date	:	
Date of last update	:	22.04.2004
Number of pages	:	20
Chapter (profile)	:	Chapter: 2, 3, 4, 5, 9
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

2.1 MELTING POINT

Value : 106 - 107 °C
Sublimation :
Method :
Year : 2000
GLP :
Test substance :

Test substance : CAS 104-15-4 (p-toluenesulphonic acid), anhydrous.
Reliability : (2) valid with restrictions
07.07.2003 (1)

Value : 107 °C
Sublimation :
Method :
Year : 1996
GLP :
Test substance :

Test substance : CAS 104-15-4 (p-toluenesulphonic acid).
Reliability : (2) valid with restrictions
07.07.2003 (2)

Value : 102 °C
Sublimation :
Method : other: calculated
Year :
GLP :
Test substance :

Test substance : CAS 104-15-4 (p-toluenesulphonic acid).
Reliability : (2) valid with restrictions
07.07.2003 (3)

2.2 BOILING POINT

Value : 140 °C at 26.7 hPa

Test substance : CAS 104-15-4 (p-toluenesulphonic acid).
Reliability : (2) valid with restrictions
07.07.2003 (1) (2)

Value : 332 °C at 1013 hPa
Decomposition :
Method : other: calculated
Year :
GLP :
Test substance :

Test substance : CAS 104-15-4 (p-toluenesulphonic acid).
Reliability : (2) valid with restrictions
07.07.2003 (3)

2.3 DENSITY

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : .0000039 hPa at 25 °C
Decomposition :
Method : other (calculated)
Year :
GLP :
Test substance :

Test substance : CAS 104-15-4 (p-toluenesulphonic acid).
Reliability : (2) valid with restrictions
07.07.2003 (3)

2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water
Log pow : -.62 at °C
pH value :
Method : other (calculated)
Year :
GLP :
Test substance :

Test substance : CAS 104-15-4 (p-toluenesulphonic acid).
Reliability : (2) valid with restrictions
07.07.2003 (3)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : ca. 670 g/l at °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method :
Year : 2000
GLP :
Test substance :

Test substance : CAS 104-15-4 (p-toluenesulphonic acid).
Reliability : (2) valid with restrictions
07.07.2003 (1)

Solubility in : Water
Value : 202.3 g/l at °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :

pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	
Remark	:	An experimental value of 620 g/L is reported. (original source: Budavari, S. (1989))
Test substance	:	CAS 104-15-4 (p-toluenesulphonic acid).
Reliability	:	(2) valid with restrictions

07.07.2003 (3)

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

Memo	:	Calculated pKa
Remark	:	The pKa was calculated to be -2.58.
Reliability	:	(2) valid with restrictions

07.07.2003 (4)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000 molecule/cm³
Rate constant	:	= .0000000000013643 cm³/(molecule*sec)
Degradation	:	= 50 % after 7.8 day(s)
Deg. product	:	
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	

Remark :

AOP Program (v1.90) Results:
==========
SMILES : O=S(=O)(O)c(ccc(c1)C)c1
CHEM : Benzenesulfonic acid, 4-methyl-
MOL FOR: C7 H8 O3 S1
MOL WT : 172.20
---------- SUMMARY (AOP v1.90): HYDROXYL RADICALS ----------
Hydrogen Abstraction = 0.1360 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.1400 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
**Addition to Aromatic Rings = 1.0883 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 1.3643 E-12 cm3/molecule-sec
HALF-LIFE = 7.840 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 94.080 Hrs
..... ** Designates Estimation(s) Using ASSUMED Value(s)
---------- SUMMARY (AOP v1.90): OZONE REACTION ----------

****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)

Test substance	:	CAS 104-15-4 (p-toluenesulphonic acid).
Reliability	:	(2) valid with restrictions

07.07.2003 (3)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	at °C
t1/2 pH7	:	at °C
t1/2 pH9	:	at °C

Remark	:	p-Toluenesulphonic acid does not contain any hydrolysable groups. It only ionizes in water. (Basic chemical knowledge)
Test substance	:	CAS 104-15-4 (p-toluenesulphonic acid).
Reliability	:	(2) valid with restrictions

19.04.2004

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 III
Media :
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: calculated
Year :

Remark :

Level III Fugacity Model (Full-Output):
==========

Chem Name : Benzenesulfonic acid, 4-methyl-
Molecular Wt: 172.2
Henry's LC : 2.78e-009 atm-m3/mole (Henrywin program)
Vapor Press : 9.57e-005 mm Hg (Mpbpwin program)
Liquid VP : 0.000549 mm Hg (super-cooled)
Melting Pt : 102 deg C (Mpbpwin program)
Log Kow : -0.62 (Kowwin program)
Soil Koc : 0.0984 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	3.18e-006	188	0
Water	99.8	360	1000
Soil	0.000914	360	0
Sediment	0.167	1.44e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.54e-017	4.01e-005	0.000109	4.01e-006	1.09e-005
Water	2.76e-014	658	342	65.8	34.2
Soil	9.28e-018	0.00603	0	0.000603	0
Sediment	2.3e-014	0.275	0.0114	0.0275	0.00114

Persistence Time: 342 hr
Reaction Time: 520 hr
Advection Time: 1e+003 hr
Percent Reacted: 65.8
Percent Advected: 34.2

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 188.2
Water: 360
Soil: 360

Sediment: 1440
Biowin estimate: 2.886 (weeks)

Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

Test substance : CAS 104-15-4 (p-toluenesulphonic acid).
Reliability : (2) valid with restrictions
11.07.2003 (3)

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic
Inoculum : activated sludge, industrial, adapted
Concentration : 100 mg/l related to Test substance
related to
Contact time :
Degradation : 90 (±) % after 24 hour(s)
Result :
Deg. product :
Method : other: activated sludge degradability test
Year : 1988
GLP : no data
Test substance :

Method : Aeration, neutral pH, 10 day adaptation, parameter: TOC
Result : 90% TOC removal
Test substance : CAS 104-15-4 (p-toluenesulphonic acid), purity not indicated.
Reliability : (4) not assignable
The information was limited to the above mentioned.
26.06.2003 (5)

Type : aerobic
Inoculum : activated sludge, adapted
Concentration : 200 mg/l related to COD (Chemical Oxygen Demand)
related to
Deg. product :
Method : other: not indicated
Year : 1976
GLP : no
Test substance :

Method : INOCULUM
- Inoculum: 100 mg/L adapted activated sludge
- Source: sewage plant
- Preparation of inoculum: daily 200 ml is separated from the 1L solution and after sedimentation the residue (200 ml) is diluted with tap water, 600 mg/L starch or glucose, 600 mg/L peptone and 25 ml phosphate buffer pH 7.2 and the tested compound; the concentration of test substance is gradually increased to 200 mg/L COD after 20 days

TEST SYSTEM

- Preparation of test solution: test substance is dissolved in medium
- Initial test substance concentration: 200 mg/L COD
- Culturing apparatus: beakers
- Number of culture flasks per concentration: 1 for test substance + inoculum + medium, 1 blank with inoculum and medium only
- Aeration: no
- Test duration: at least 120 h
- Sampling: once or twice daily
- Analytical parameter: COD

TEST CONDITIONS
- Composition of mineral solution: 27.5 mg CaCl2, 22.5 mg MgSO4.7H2O, 0.25 mg ferric chloride.6H2O, 50 mg ammonium sulphate, 20 ml of phosphate buffer (pH 7.2) and 100 ml tap water in distilled water
- Test temperature: 20 ± 3 °C

REFERENCE SUBSTANCE: 200 mg/L aniline based on COD

Result : Percentage biodegradation corrected for blank: 98.7 based on COD.
Rate of biodegradation: 8.4 mg COD/g/h.

REFERENCE SUBSTANCE
Percentage biodegradation corrected for blank: 94.5 based on COD.
Rate of biodegradation: 19.0 mg COD/g/h.

Test substance : CAS 104-15-4 (p-toluenesulphonic acid), purity not indicated.

Reliability : (4) not assignable
1. The information is limited to the above mentioned.
2. The study is performed with adapted sludge, which is not allowed according to OECD guidelines.

08.07.2003 (6)

Type : aerobic
Inoculum :
Concentration : .6 g/l related to COD (Chemical Oxygen Demand)
related to
Contact time :
Degradation : 44 (±) % after
Result :
Deg. product :
Method : other: not indicated
Year : 1972
GLP : no
Test substance :

Remark : COD 1560 mg O2/g
BOD 1030 mg O2/g

Degradation (= reduction of COD): 44%

Test substance : CAS 104-15-4 (p-toluenesulphonic acid), purity pro analyse.

Reliability : (4) not assignable
The information is limited to the above mentioned.

07.07.2003 (7)

Type : aerobic
Inoculum :
Contact time :
Degradation : > 90 (±) % after 5 day(s)
Result :
Deg. product :
Method : other: not indicated
Year : 1978
GLP : no

Test substance	:	
Remark	:	Organic carbon 450 mg/g ThOD 1672 mg O2/g COD 1480 mg O2/g BOD 380 mg O2/g COD-elimination: >90% after 5 days
Test substance	:	CAS 104-15-4 (p-toluenesulphonic acid), purity not indicated.
Reliability	:	(4) not assignable The information is limited to the above mentioned.
07.07.2003		(8)
Type	:	aerobic
Inoculum	:	
Contact time	:	
Degradation	:	100 (±) % after 5 day(s)
Result	:	
Deg. product	:	
Method	:	other: not indicated
Year	:	1983
GLP	:	no data
Test substance	:	
Remark	:	DOC 360 mg C/g COD 1040 mg O2/g BOD 300 mg O2/g Degradation was 10% after 3 hours and 100% after 5 days.
Test substance	:	CAS 104-15-4 (p-toluenesulphonic acid), purity 65%.
Reliability	:	(4) not assignable The information is limited to the above mentioned.
07.07.2003		(9)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	static
Species	:	Leuciscus idus melanotus (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	> 325
Limit test	:	no
Analytical monitoring	:	no
Method	:	other: not indicated
Year	:	1981
GLP	:	no
Test substance	:	

Method :

TEST ORGANISMS
- Species: Leuciscus idus f. melanotus
- Supplier: Paul Eggers, 2345 Hohenwestedt
- Size/weight/loading: 5.5-6.6 cm/1.5-2.7 g/0.75-1.35 g/L
- Feeding (pretreatment): Tetra Min

STOCK AND TEST SOLUTION AND THEIR PREPARATION
Test substance was dissolved in medium and added to the solution in the aquarium.

DILUTION WATER
- Source: deionised tapwater
- Hardness: 114 mg CaCO3/l
- Ca/Mg ratio: 0.7
- Na/K ratio: 21
- pH (after aeration with fish): 8.0-8.2
- O2: >7 mg/L
- Conductance: <5 µS/cm

TEST SYSTEM
- Test type: static
- Concentrations: 0, 10, 100 and 500 mg/L
- Exposure vessel type: glass aquarium (40x25x30 cm) containing 20 liter of solution
- Number of fish: 10 per replicate, 1 replicate/treatment
- Photoperiod: 12 hours (700 lux)
- Test duration: 96 hours
- Test parameter: mortality
- Observation times: regularly
- Aeration: yes

PHYSICAL MEASUREMENTS
- Measuring times: 0, 2, 24, 48, 72 and 96 hours for pH, dissolved oxygen and temperature
- Test temperature: 20 ± 1 °C
- Dissolved oxygen: 8.5-9.2 mg/L
- pH: 7.5-8.2 (at 500 mg/L 5.7 after 2 hours and still slightly decreased after 24, 48 and 96 hours)

Result :

RESULTS
- Mortality: none
- Other effects: no difference in behaviour compared to control group; macroscopic examination showed no changes

Test substance : CAS 104-15-4 (p-toluenesulphonic acid), purity 65% in water.

Conclusion : The LC50 >500 mg/L, which is equivalent to >325 mg/L (p-toluenesulphonic acid is a 65% solution in water).

Reliability	:	(2) valid with restrictions The method used is predominantly according to OECD203, except that Leuciscus idus melanotus is not a recommended species, only 4 concentrations were tested and no analyses were performed.
07.07.2003		(10)
Type	:	other: not indicated
Species	:	Lebistes reticulatus (Fish, fresh water)
Exposure period	:	48 hour(s)
Unit	:	mg/l
LC0	:	> 500
Limit test	:	
Analytical monitoring	:	no data
Method	:	other: not indicated
Year	:	1972
GLP	:	no
Test substance	:	
Test substance	:	CAS 104-15-4 (p-toluenesulphonic acid), purity pro analyse.
Reliability	:	(4) not assignable The information is limited to the above mentioned.
07.07.2003		(7)
Type	:	other: not indicated
Species	:	Leuciscus idus (Fish, fresh water)
Exposure period	:	
Unit	:	mg/l
LC0	:	= 200
Limit test	:	
Analytical monitoring	:	no data
Method	:	other: not indicated
Year	:	1978
GLP	:	no
Test substance	:	
Test substance	:	CAS 104-15-4 (p-toluenesulphonic acid), purity not indicated.
Reliability	:	(4) not assignable The information is limited to the above mentioned.
07.07.2003		(8)
Type	:	other
Species	:	
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	= 371000
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	
Test substance	:	CAS 104-15-4 (p-toluenesulphonic acid).
Reliability	:	(4) not assignable
07.07.2003		(3)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	
Species	:	Daphnia magna (Crustacea)
Exposure period	:	
Unit	:	mg/l

EC0	:	> 1625
Analytical monitoring	:	no data
Method	:	other: not indicated
Year	:	1983
GLP	:	no data
Test substance	:	

Test substance	:	CAS 104-15-4 (p-toluenesulphonic acid), purity 65%.
Conclusion	:	EC0 >2500 mg/L, which is equivalent to 1625 mg/L for the substance tested (65%).
Reliability	:	(4) not assignable The information is limited to the above mentioned.

07.07.2003 (9)

Type	:	other
Species	:	Daphnia sp. (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
EC50	:	= 331000
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	

Test substance	:	CAS 104-15-4 (p-toluenesulphonic acid).
Reliability	:	(4) not assignable

07.07.2003 (3)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	other algae: green algae
Endpoint	:	
Exposure period	:	96 hour(s)
Unit	:	g/l
EC50	:	= 178
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	

Test substance	:	CAS 104-15-4 (p-toluenesulphonic acid).
Reliability	:	(4) not assignable

07.07.2003 (3)

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	:	= 1410 mg/kg bw
Species	:	rat
Strain	:	Wistar
Sex	:	male/female
Number of animals	:	5
Vehicle	:	
Doses	:	1250, 1600 and 2000 mg/kg for females and 2000 mg/kg for males
Method	:	OECD Guide-line 401 "Acute Oral Toxicity"
Year	:	1988
GLP	:	yes
Test substance	:	

Method :

TEST ANIMALS:
- Source: Hoechst AG
- Age: male ca. 7 weeks, female ca. 8 weeks
- Number: 5/sex/dose
- Weight at study initiation: male 194-202 g; female 181-196 g

ADMINISTRATION
- Route: oral (gavage)
- Doses: 1250, 1600 and 2000 mg/kg for females and 2000 mg/kg for males
- Volume administered or concentration: 10 ml/kg

EXAMINATIONS: mortality and clinical symptoms several times on day 1 and daily thereafter; body weight weekly; macroscopic examination of animals found dead and sacrificed; post-exposure period was 28 days.

STATISTICAL METHOD: Probit-analysis

Result :

MORTALITY
- Number of deaths at each dose: 2/5, 3/5 and 4/5 at 1250, 1600 and 2000 mg/kg for females and 2/5 at 2000 mg/kg for males
- Time of death: on day 1, except for 1 animal at 1600 mg/kg died on day 13

BODY WEIGHT: decreased body weight during post-exposure period.

MAIN CLINICAL SIGNS:
Hypoactivity, hunched posture, emaciation, irregular breathing were observed in all animals from all dose groups on day 1 and reversible within 3 days for males at 2000 mg/kg. In males at 2000 mg/kg some of the symptoms re-occurred in 1 or 2 animals after 14 days. For females at 1250 mg/kg the above symptoms were reversible within 2 days. For females at 1600 and 2000 mg/kg some of the symptoms were irreversible in 1-2 animals.
Abnormal gait, ptosis and piloerection were seen in several animals from all dose groups on day 1. Symptoms were reversible within 2 days for males at 2000 mg/kg and for females at 1250 mg/kg; some symptoms re-occurred within the 28-day observation period. For females at 1600 and 2000 mg/kg ptosis, piloerection and abnormal gait were observed during the 28 days observation period.

NECROPSY FINDINGS:
Red discolouration of the GI tract filled with blood, white discolouration of the mucosa of the stomach and intestine, pale adrenals, growing together of stomach and nearby organs, stomach haemorrhages and abdomen filled with fluid (in animals that died spontaneously).

SEX-SPECIFIC DIFFERENCES: none

Test substance : CAS 104-15-4 (p-toluenesulphonic acid), purity >98%.
Reliability : (1) valid without restriction
02.04.2004 (11)

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

Species : rabbit
Concentration : 500 mg
Exposure : Semiocclusive
Exposure time : 4 hour(s)
Number of animals : 1
Vehicle : physiol. saline
PDII :
Result : corrosive
Classification : corrosive (causes burns)
Method : OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year : 1988
GLP : yes
Test substance :

Method : TEST ANIMALS
- Strain: New Zealand white rabbit
- Sex: not indicated
- Age: ca. 3-5 months
- Weight at study initiation: 2.0-2.6 kg
- Number of animals: 1 (3 animals were exposed for 3 minutes)

ADMINISTRATION/EXPOSURE
- Preparation of test substance: 500 mg wetted with 0.1 ml 0.9% saline
- Area of exposure: 6.25 cm2
- Occlusion: semiocclusion
- Removal of test substance: with water after exposure

EXAMINATIONS
- Scoring system: Draize
- Observation times: 30-60 minutes, 24, 48 and 72 hours, and 7 days after exposure for 4 hours exposure only

Result : 4-hour exposure:
AVERAGE SCORE (24-72 h)
- Erythema: 3.7
- Edema: 2

REVERSIBILITY: not reversible within 7 days

OTHER EFFECTS: dry, fissured skin, eschar formation, brown discolouration; scar formation and open wound after 7 days

3-minute exposure:
AVERAGE SCORE (24-72 h)
- Erythema: 0.6
- Edema: 0

REVERSIBILITY: within 72 hours

OTHER EFFECTS: brown discolouration

Test substance : CAS 104-15-4 (p-toluenesulphonic acid), purity >98%.
Reliability : (1) valid without restriction
22.03.2004 (12)

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

Type	:	Sub-acute
Species	:	rat
Sex	:	male/female
Strain	:	Wistar
Route of admin.	:	oral unspecified
Exposure period	:	28 days
Frequency of treatm.	:	daily; 7 times/week
Post exposure period	:	
Doses	:	0, 4, 20, 100, 500 mg/kg bw/d
Control group	:	yes
NOAEL	:	> 500 mg/kg bw
Method	:	OECD Guide-line 407 "Repeated Dose Oral Toxicity - Rodent: 28-day or 14-d Study"
Year	:	1990
GLP	:	yes
Test substance	:	
Result	:	In the highest dose group urine was acidic in both sexes and in males a higher saliva production at the end of the study was observed.
Test substance	:	CAS 104-15-4 (p-toluenesulphonic acid), purity not indicated.
Conclusion	:	The findings observed at 500 mg/kg are not considered to be toxicologically relevant. NOEL = 100 mg/kg.
Reliability	:	(4) not assignable Secondary literature. The information given was limited to the above mentioned.

22.04.2004 (13)

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Ames test
System of testing	:	Salmonella typhimurium TA98, TA100, TA1535, TA1537 and TA1538
Test concentration	:	0, 10, 100, 500, 1000 and 5000 µg/plate

Cytotoxic concentr.	:	>5000 µg/plate
Metabolic activation	:	with and without
Result	:	negative
Method	:	OECD Guide-line 471
Year	:	1988
GLP	:	yes
Test substance	:	

Method :

TEST SYSTEM
- Species/cell type: Salmonella typhimurium TA98, TA100, TA1535, TA1537 and TA1538
- Deficiency: histidine
- Metabolic activation system: Aroclor 1254 rat liver S9-mix

ADMINISTRATION
- Dosing: 0, 10, 100, 500, 1000 and 5000 µg/plate
- Number of replicates: 3
- Application: plate incorporation
- Positive control groups: sodium azide (without S9; TA1535 and TA100); 9-aminoacridine (without S9; TA1537); 2-nitrofluorene (without S9; TA1538 and TA98); 2-aminofluorene (with S9; TA1538 and TA98).
- Negative control group: distilled water

DEVIATIONS FROM GUIDELINE: no positive controls were used for TA100, TA1535 and TA1537 with metabolic activation; however, the number of revertants is very low.

Result :

GENOTOXIC EFFECTS
- With metabolic activation: negative
- Without metabolic activation: negative

PRECIPITATION CONCENTRATION: >5000 µg/plate

CYTOTOXIC CONCENTRATION
- With metabolic activation: >5000 µg/plate
- Without metabolic activation: >5000 µg/plate

Test substance	:	CAS 104-15-4 (p-toluenesulphonic acid), purity >98%.
Reliability	:	(1) valid without restriction 1. As no E-coli strain was included in the study design some base-pair substitutions may remain undiscovered. 2. The number of cells/culture were not specified.

07.07.2003 (14)

Type	:	Chromosomal aberration test
System of testing	:	V79 Chinese hamster cells
Test concentration	:	0, 200, 600 and 1902 µg/ml
Cytotoxic concentr.	:	>1902 µg/ml
Metabolic activation	:	with and without
Result	:	negative
Method	:	OECD Guide-line 473
Year	:	1988
GLP	:	yes
Test substance	:	

Method :

TEST SYSTEM
- Species/cell type: V79 Chinese hamster cells
- Metabolic activation system: Aroclor 1254 induced rat liver S9-mix
- No. of metaphases analyzed: 100

ADMINISTRATION
- Dosing: 0, 200, 600 and 1902 µg/ml
- Number of replicates: 2

- Application: in bidest water
- Positive control group: ethylmethanesulfonate (without S9), cyclophosphamide (with S9)
- Negative control groups: bidest water and untreated
- Pre-incubation time: 24 hours
- Incubation time: 2 hours
- Fixation interval: 6, 18 and 28 hours for 1902 µg/ml and 18 hours for 200 and 600 µg/ml (last 2.5 hours Colcemid was added)

CRITERIA FOR EVALUATING RESULTS
classified as mutagenic if the test substance induces a significantly increased aberration rate as compared with the negative controls with one of the concentrations tested and if there is a reproducible concentration related increase in the aberration rate.

Result : GENOTOXIC EFFECTS
- With metabolic activation: negative
- Without metabolic activation: negative

FREQUENCY OF EFFECTS (excluding gaps)
without S9: 2, 0.5 and 0% at 200, 600 and 1902 µg/ml after 18 hours; 2% at 1902 µg/ml after 28 hours
with S9: 2.5, 2 and 0.5% at 200, 600 and 1902 µg/ml after 18 hours; 0.5% at 1902 µg/ml after 28 hours

PRECIPITATION CONCENTRATION: >1902 µg/ml (= 10 mM)

MITOTIC INDEX: Concentration-related plating efficiency was established in 1000 cells from each of two slides per test group. No influence on mitotic index was observed.

CYTOTOXIC CONCENTRATION
- With metabolic activation: >1902 µg/ml
- Without metabolic activation: >1902 µg/ml

Test substance : CAS 104-15-4 (p-toluenesulphonic acid), purity >98%.

Reliability : (1) valid without restriction

07.07.2003 (15)

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

(1) Merck Index, CD-rom 2000.

(2) SAX's Dangerous Properties of Industrial Materials, (Ed. R.J. Lewis Sr., 9th Ed., Van Nostrand Reinhold, NY, 1996, p. 3195.

(3) EPISuite v.3.10, April 2001.

(4) Pallas 2.1, 1994/95.

(5) Matsui, S.; Y. Okawa & R. Ota, Experience of 16 years' operation and maintenance of the Fukashiba industrial wastewater treatment plant of the Kashima petrochemical complex - II. Biodegradability of 37 organic substances and 28 process wastewaters, Water Sci. Technol. 20: 201-210, 1988.

(6) Pitter, P., Determination of biological degradability of organic substances, Water Res. 10: 231-235, 1976.

(7) Hoechst AG, internal report (07.12.1972).

(8) Hoechst AG, internal report (31.08.1978).

(9) Hoechst AG, internal report, Bericht W82-360 (23.3.1983).

(10) Hoechst AG, Akute Toxizitaet von p-Toluolsulfonsaeure Loesung 65%ig an Goldorfen, Bericht 197/81, 1981.

(11) Hoechst AG, p-Toluolsulfonsaeure: Pruefung der akuten oralen Toxizitaet an der Wistar-Ratte, Bericht 88.1563, 1988.

(12) Hoechst AG, p-Toluolsulfonsäure: Prüfung auf Hautreizung am Kaninchen, Bericht 88.1576, 1988.

(13) Hoechst AG (1990): Internal report No. 90.0037 in IUCLID Dataset Toluene-4-sulphonic acid (CAS No. 104-15-4) on IUCLID CD-ROM, 2000.

(14) Hoechst AG, EXT 8804 p-Toluenesulfonic acid: Reverse mutation assay in vitro Ames test, Bericht 88.0892, 1988.

(15) Hoechst AG, p-Toluolsulfonsaeure: Chromosome aberrations in vitro in V79 chinese hamster cells, Report No. 88.1940, 1988.

Appendix 2

I U C L I D

Data Set

Existing Chemical	:	ID: 98-11-3
CAS No.	:	98-11-3
EINECS Name	:	benzenesulphonic acid
EC No.	:	202-638-7
TSCA Name	:	benzenesulfonic acid

Producer related part

Company	:	Notox
Creation date	:	14.04.2003

Substance related part

Company	:	Notox
Creation date	:	14.04.2003
Status	:	
Memo	:	
Printing date	:	03.07.2006
Revision date	:	
Date of last update	:	08.06.2005
Number of pages	:	20
Chapter (profile)	:	Chapter: 2, 3, 4, 5, 9
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

2.1 MELTING POINT

Value : = 43 - 44 °C
Sublimation :
Method :
Year : 1996
GLP :
Test substance :

Test substance : CAS 98-11-3 (benzenesulphonic acid).
Reliability : (2) valid with restrictions
04.06.2003 (1)

Value : = 50 - 51 °C
Sublimation :
Method :
Year : 2000
GLP :
Test substance :

Remark : Also reported: 65-66 °C for anhydrous and 43-44 °C for sesquihydrate.
Test substance : CAS 98-11-3 (benzenesulphonic acid), anhydrous.
Reliability : (2) valid with restrictions
04.06.2003 (2)

Value : = 89 °C
Sublimation :
Method : other: calculated
Year :
GLP :
Test substance :

Test substance : CAS 98-11-3 (benzenesulphonic acid).
Reliability : (2) valid with restrictions
07.07.2003 (3)

2.2 BOILING POINT

Value : 171 - 172 °C at .13 hPa

Remark : Using NOMO5 (Mitre Corporation, Version 2.0, 12/4/87), this measured boiling point is estimated to amount to 403 deg C at atmospheric pressure.
Test substance : CAS 98-11-3 (benzenesulphonic acid).
Reliability : (2) valid with restrictions
19.04.2004 (4)

Value : = 319 °C at 1013 hPa
Decomposition :
Method : other: calculated
Year :
GLP :
Test substance :

Test substance : CAS 98-11-3 (benzenesulphonic acid).
Reliability : (2) valid with restrictions
28.04.2003 (3)

2.3 DENSITY

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	= .0000000022 - .0000047 hPa at 20 °C
Decomposition	:	
Method	:	OECD Guide-line 104 "Vapour Pressure Curve"
Year	:	2004
GLP	:	yes
Test substance	:	
Remark	:	The lower value was calculated from the boiling temperature resulting from the NOMO5 estimation on the measured boiling temperature. The higher value was calculated from the boiling temperature from EPISuite.
Test substance	:	CAS 98-11-3 (benzenesulphonic acid).
Reliability	:	(1) valid without restriction

28.04.2004 (5)

Value	:	= .0000228 hPa at 25 °C
Decomposition	:	
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	
Test substance	:	CAS 98-11-3 (benzenesulphonic acid).
Reliability	:	(2) valid with restrictions

28.04.2003 (3)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	= -1.17 at °C
pH value	:	
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	
Test substance	:	CAS 98-11-3 (benzenesulphonic acid).
Reliability	:	(2) valid with restrictions

24.04.2003 (3)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	at °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	.7 at 25 °C

Description	:	
Stable	:	
Deg. product	:	
Method	:	
Year	:	2000
GLP	:	
Test substance	:	

Test substance	:	CAS 98-11-3 (benzenesulphonic acid).
Reliability	:	(2) valid with restrictions

04.06.2003 (2)

Solubility in	:	Water
Value	:	= 689.5 g/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	

Test substance	:	CAS 98-11-3 (benzenesulphonic acid).
Reliability	:	(2) valid with restrictions

07.07.2003 (3)

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

Memo	:	Calculated pKa
Remark	:	The pKa was calculated to be -2.80.

Reliability : (2) valid with restrictions
24.04.2003 (6)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000 molecule/cm³
Rate constant	:	= .0000000000005569 cm³/(molecule*sec)
Degradation	:	= 50 % after 19.2 day(s)
Deg. product	:	
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	

Remark :

AOP Program (v1.90) Results:
==========
SMILES : O=S(=O)(O)c(cccc1)c1
CHEM : Benzenesulfonic acid
MOL FOR: C6 H6 O3 S1
MOL WT : 158.17
---------- SUMMARY (AOP v1.90): HYDROXYL RADICALS ----------
Hydrogen Abstraction = 0.0000 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.1400 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
**Addition to Aromatic Rings = 0.4169 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 0.5569 E-12 cm3/molecule-sec
HALF-LIFE = 19.207 Days (12-hr day; 1.5E6 OH/cm3)
..... ** Designates Estimation(s) Using ASSUMED Value(s)
---------- SUMMARY (AOP v1.90): OZONE REACTION ----------

****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)

Test substance	:	CAS 98-11-3 (benzenesulphonic acid).
Reliability	:	(2) valid with restrictions

07.07.2003 (3)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	at °C
t1/2 pH7	:	at °C
t1/2 pH9	:	at °C

Remark	:	Benzene sulphonic acid does not contain any hydrolysable groups. It only ionizes in water. (Basic chemical knowledge)
Test substance	:	CAS 98-11-3 (benzenesulphonic acid).
Reliability	:	(2) valid with restrictions

19.04.2004

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

Type of measurement	:	other: concentration at possibly contaminated sites
Media	:	surface water
Concentration	:	
Method	:	sequential solid-phase extraction followed by ion-pair liquid chromatography coupled to electrospray ionisation-mass spectrometry
Method	:	Aliquots of coastal water from two submarine outfalls located at the river mouths of the Besos and the Llobregat near Barcelona were analysed by means of sequential solid-phase extraction followed by ion-pair liquid chromatography coupled to electrospray ionisation-mass spectrometry. Samples were taken bimonthly from March 1999 - July 2000. Nine samples were taken in each specific point.
Result	:	Only in May 1999 a concentration of 1.81-5.35 ng/ml of benzenesulphonic acid was detected in Barcelona coastal waters; the other months amounts were below the limit of detection.
Test substance	:	CAS 98-11-3 (benzenesulphonic acid).
Reliability	:	(2) valid with restrictions

24.04.2003 (7)

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level III
Media	:	
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: calculated
Year	:	
Remark	:	

Level III Fugacity Model (Full-Output):

==========

Chem Name : Benzenesulfonic acid
Molecular Wt: 158.17
Henry's LC : 2.52e-009 atm-m3/mole (Henrywin program)
Vapor Press : 0.000312 mm Hg (Mpbpwin program)
Liquid VP : 0.00133 mm Hg (super-cooled)
Melting Pt : 88.8 deg C (Mpbpwin program)
Log Kow : -1.17 (Kowwin program)
Soil Koc : 0.0277 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	2.62e-006	461	0
Water	99.8	360	1000
Soil	0.00083	360	0
Sediment	0.166	1.44e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.38e-017	1.35e-005	8.97e-005	1.35e-006	8.97e-006
Water	2.72e-014	658	342	65.8	34.2
Soil	8.37e-018	0.00547	0	0.000547	0
Sediment	2.27e-014	0.274	0.0114	0.0274	0.00114

Persistence Time: 342 hr
Reaction Time: 520 hr
Advection Time: 1e+003 hr
Percent Reacted: 65.8
Percent Advected: 34.2

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 461
Water: 360
Soil: 360
Sediment: 1440
Biowin estimate: 3.014 (weeks)

Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

Test substance : CAS 98-11-3 (benzenesulphonic acid).
Reliability : (2) valid with restrictions
11.07.2003 (3)

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic
Inoculum : activated sludge, adapted
Concentration : 200 mg/l related to COD (Chemical Oxygen Demand) related to
Deg. product :
Method : other: not indicated
Year : 1976
GLP : no
Test substance :

Method : INOCULUM
- Inoculum: 100 mg/L adapted activated sludge
- Source: sewage plant
- Preparation of inoculum: daily 200 ml is separated from the 1L solution and after sedimentation the residue (200 ml) is diluted with tap water, 600 mg/L starch or glucose, 600 mg/L peptone and 25 ml phosphate buffer pH 7.2 and the tested compound; the concentration of test substance is gradually increased to 200 mg/L COD after 20 days

TEST SYSTEM
- Preparation of test solution: test substance is dissolved in medium
- Initial test substance concentration: 200 mg/L COD
- Culturing apparatus: beakers

- Number of culture flasks per concentration: 1 for test substance + inoculum + medium, 1 blank with inoculum and medium only
- Aeration: no
- Test duration: at least 120 h
- Sampling: once or twice daily
- Analytical parameter: COD

TEST CONDITIONS
- Composition of mineral solution: 27.5 mg CaCl2, 22.5 mg MgSO4.7H2O, 0.25 mg ferric chloride.6H2O, 50 mg ammonium sulphate, 20 ml of phosphate buffer (pH 7.2) and 100 ml tap water in distilled water
- Test temperature: 20 ± 3 °C

REFERENCE SUBSTANCE: 200 mg/L aniline based on COD

Result : Percentage biodegradation corrected for blank: 98.5 based on COD.
Rate of biodegradation: 10.6 mg COD/g/h.

REFERENCE SUBSTANCE
Percentage biodegradation corrected for blank: 94.5 based on COD.
Rate of biodegradation: 19.0 mg COD/g/h.

Test substance : CAS 98-11-3 (benzenesulphonic acid), purity not indicated.

Reliability : (4) not assignable
1. The information is limited to the above mentioned.
2. The study is performed with adapted sludge, which is not allowed according to OECD guidelines.

08.07.2003 (8)

Type : aerobic
Inoculum : other: soil microorganisms
Concentration : 100 mg/l related to Test substance
related to
Deg. product :
Method : other: not indicated
Year : 1966
GLP : no
Test substance :

Method : INOCULUM/TEST ORGANISM
- Inoculum: 1.0 ml of 1% suspension of Niagara silt loam

TEST SYSTEM
- Initial test substance concentration: 45.5 mg C/L
- Culturing apparatus: 45 mm diameter X 80 mm high screw-cap bottles containing 40 ml of medium
- Number of culture flasks per concentration: 2 for test substance + inoculum; 2 for test substance + inoculum + HgCl2; 2 for 1% glucose controls
- Measuring equipment: Beckman spectrophotometer
- Test duration: 64 days
- Sampling: samples were taken after mixing, at intervals of 3 to 6 hours and at 1, 2, 4, 8, 16, 32 and 64 days after inoculation
- Analytical parameter: absorbance at 264 nm relative to soil-medium mixture without chemical

TEST CONDITIONS
- Composition of mineral solution: 1.6 g K2HPO4, 0.40 g KH2PO4, 0.50 g NH4NO3, 0.20 g MgSO4.7H2O, 25 mg CaCl2.2H2O, 2.3 mg FeCl3.6H2O in 1 L of distilled water
- Test temperature: 25 °C

Result : The time necessary for complete degradation was established to be 16 days. The degradation was due to biological activity, because no

decreased absorbance was seen in vessels with HgCl2.

Test substance : CAS 98-11-3 (benzenesulphonic acid), purity not indicated.
Reliability : (4) not assignable
The information was limited to the above mentioned.

22.04.2003 (9)

Type : aerobic
Inoculum :
Deg. product :
Method :
Year : 1980
GLP :
Test substance :

Remark : Two hundred sixty of the existing chemicals listed by MITI have been tested for biodegradability; a structure-activity relationship could be deduced for some groups.
Benzenesulphonic acid is reported to be degradable, although the presence of the sulfonic acid-group was indicated to decrease the degradability of aromatic substances.
Test substance : CAS 98-11-3 (benzenesulphonic acid), purity not indicated.
Reliability : (4) not assignable
03.06.2003 (10)

Type : anaerobic
Inoculum : other: aquifer microorganisms
Concentration : .2 mmol/l related to Test substance
related to
Contact time : 13 month
Degradation : (±) % after
Result :
Deg. product :
Method : other: not indicated
Year : 1989
GLP : no data
Test substance :

Remark : The test substance was inoculated with aquifer slurry from two sites near a municipal landfill: a methanogenic site (TOC 288 mg/L and sulfate concentration < 0.1 mM) and a sulfate reducing site (TOC 14.4 mg/L and sulfate concentration 2.1 mM). Experiments were performed in the dark at room temperature in duplicate with sterilised aquifer slurries as control. Disappearance of the test substance was analysed by reversed-phase HPLC with UV detection at 264 nm.

Results:
Sulphate-reducing slurry (0, 13 months): 205, 198 µM
Methanogenic slurry (0, 13 months): 204, 196 µM
Test substance : CAS 98-11-3 (benzenesulphonic acid), purity not indicated.
Conclusion : No biodegradation was observed for p-hydroxybenzenesulphonic acid.
Reliability : (4) not assignable
22.04.2003 (11)

Type : anaerobic
Inoculum : other: laboratory-made sludge
Concentration : 100 mg/l related to DOC (Dissolved Organic Carbon)
related to
Deg. product :
Method : other: not indicated
Year : 1999
GLP : no data

Test substance	:	
Remark	:	Benzenesulphonic acid was anaerobically incubated with 10 ml of laboratory-made sludge suspension (TOC 158.6 mg/L) at 37 °C for 8 weeks. The gas volume produced was very similar to that of the blank and the test substance was classified as persistent. Benzenesulphonic acid at the concentration used (100 mgC/L) was slightly inhibitory (<=25%) to the microorganisms used. Benzene sulphonic acid is a persistent chemical under the anaerobic degradation conditions as employed in this test.
Test substance	:	CAS 98-11-3 (benzenesulphonic acid), purity analytical grade.
Reliability	:	(4) not assignable
03.06.2003		(12)

Type	:	
Inoculum	:	other: OS-1 bacteria
Deg. product	:	
Method	:	other: not indicated
Year	:	1986
GLP	:	no data
Test substance	:	
Remark	:	A pure culture of OS-1 bacteria isolated to utilise 2-aminobenzenesulphonate as sole carbon source also degraded benzenesulphonate and 4-methylbenzenesulphonate. The respective specific growth rates are 0.11, 0.19 and 0.07 h-1.
Test substance	:	CAS 98-11-3 (benzenesulphonic acid), purity not indicated.
Reliability	:	(4) not assignable Only a summary of study is reported.
03.06.2003		(13)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	other
Species	:	
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	= 1120000
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	

Test substance	:	CAS 98-11-3 (benzenesulphonic acid).
Reliability	:	(4) not assignable

07.07.2003 (3)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	static
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
NOEC	:	>= 100
EC50	:	> 100
Analytical monitoring	:	yes
Method	:	OECD Guide-line 202
Year	:	2005
GLP	:	yes
Test substance	:	

Method :

TEST ORGANISMS
- Species: Daphnia magna (Crustacea, Cladocera)
- Source/supplier: In-house laboratory culture with a known history.
- Age: <24 hours
- Feeding (pretreatment): daily, a suspension of fresh water algae.
- Feeding during test: no feeding.

STOCK AND TEST SOLUTION AND THEIR PREPARATION
A stock solution of 100 mg/L in ISO-medium, applying 5-8 minutes of magnetic stirring.

DILUTION WATER (ISO-medium)
- Source: tap water purified by reverse osmosis.
- Hardness: 250 mg/L expressed as CaCO3.
- pH: 8.0 ± 0.2

TEST SYSTEM
- Test type: static
- Concentrations: 0, 100 mg/L
- Exposure vessel type: 100 ml, all-glass
- Number of individuals: 5 per vessel containing 80 ml test solutionreplicates (20 per concentration)
- Photoperiod (intensity of irradiation): 16 hours photoperiod daily
- Test duration: 48 h
- Test parameter: immobility (including mortality)
- Observation times: at 24 hours and at 48 hours.

PHYSICAL MEASUREMENTS
- Measuring times: pH and dissolved oxygen at the beginning and at the end of the test, for both the 100 mg/l concentration and the blank-control. Temperature of medium continuously in a temperature control vessel, beginning at the start of the test.
- Test temperature: 19.1-19.7°C
- Dissolved oxygen: 9.2-9.7 mg/L
- pH: control 7.9-8.0; 100 mg/L 5.9-7.2

ANALYSES
- Method: HPLC (RP, UV detection at 263 nm)
- Sampling times: at t=0 and t=48 h.

REFERENCE SUBSTANCE: potassium dichromate.

Result : RESULTS
- Nominal concentrations (mg/L): 0 and 100 mg/L
- Measured concentrations (mg/L): 0 (not detected) and 103 mg/L.
- Immobility: 0% and 0% at 0 and 100 mg/L.

RESULTS REFERENCE SUBSTANCE
- Concentrations: 0, 0.1, 0.18, 0.32, 0.56, 1.0 and 1.8 mg/L
- Results: 0, 0, 0, 0, 5, 100 and 100% immobile.

Test substance : CAS 98-11-3 (benzenesulphonic acid), purity 99.8%.

Reliability : (1) valid without restriction
The pH of the 100 mg/l concentration was just below 6.0 (5.9) at the start of the test but increased during the test period (7.2 at t=48 h). Since the difference was only marginal, this was not considered to have an effect on the daphnids.

08.06.2005 (14)

Type : other
Species : Daphnia sp. (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
EC50 : = 963000
Method : other: calculated
Year :
GLP :
Test substance :

Test substance : CAS 98-11-3 (benzenesulphonic acid).

Reliability : (4) not assignable

07.07.2003 (3)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species : Selenastrum capricornutum (Algae)
Endpoint : other: biomass and growth rate
Exposure period : 72 hour(s)
Unit : mg/l
NOEC : = 46
EC50 : = 73
Limit test : no
Analytical monitoring : yes
Method : OECD Guide-line 201 "Algae, Growth Inhibition Test"
Year : 2005
GLP : yes
Test substance :

Method : TEST ORGANISMS

- Species: Selenastrum capricornutum, strain: NIVA CHL 1.
- Source/supplier: in-house laboratory culture.
- Method of cultivation: according to guideline.
- Pretreatment: 3 days under test conditions
- Initial cell concentration:10000 cells/ml

STOCK AND TEST SOLUTION AND THEIR PREPARATION
A stock solution of 220 mg/L was prepared in test medium, applying 5-6 minutes of magnetic stirring. Lower test concentrations were prepared by subsequent dilutions of the stock in test medium.

DILUTION WATER
- Source: M2; according to the ISO-Standard.

GROWTH/TEST MEDIUM CHEMISTRY
- Hardness: 24 mg/L CaCO3
- pH: 8.3 ± 0.2

TEST SYSTEM
- Concentrations: 0, 4.6, 10, 22, 46, 100 and 220 mg/L
- Exposure vessel type: 100 ml, all-glass, containing 50 ml of test medium
- Number of replicates: 3 replicates of each test concentration
6 replicates of the blank-control
1 replicate of the highest concentration without algae
- Photoperiod: Continuously with a light intensity within the range of 73 to 101 uE.m-2.s-1.
- Test duration:72 h
- Test parameter: inhibition of cell growth and reduction of growth rate.
- Observation times: at t=0 h and t=72 h

PHYSICAL MEASUREMENTS
- Measuring times: pH at the beginning and at the end of the test; temperature continuously.
- Test temperature: 22.5-23.0°C
- pH:

Concentration Test substance (mg/l)	Exposure time (hours) 0	72
0 (Blank-control)	8.1	9.3
4.6	8.0	9.3
10	7.7	9.2
22	7.2	9.2
46	6.8	9.2
100	5.0	5.2
220	3.1	3.0

ANALYSES
- Method: HPLC (RP, UV detection at 263 nm)
- Sampling times: at t=0 and t=72 h.

REFERENCE SUBSTANCE: Potassium dichromate

STATISTICAL METHOD: log-linear regression analysis

Result **:** RESULTS
- Nominal concentrations (mg/L): 0, 4.6, 10, 22, 46, 100 and 220 mg/L
- Mean measured concentrations (mg/L): 0 (not detected), 4.3, 10.1, 21.9, 44.8, 101, 224 and 233 mg/L.
- Cell density data: 111, 112, 105, 113, 118, 2.1 and 1.1 cells*10000/mL at 0, 4.6, 10, 22, 46, 100 and 220 mg/L.
- Inhibition growth rate (% of control): 0, -0.3, 1.0, -0.4, -1.3, 84 and 98.
- Inhibition biomass (AUC) (% of control): 0, 0.5, 5.9, 1.3, -4.6, 97 and 100.

GROWTH FACTOR CONTROL: 27.6

RESULTS REFERENCE SUBSTANCE
- Concentrations: 0, 0.18, 0.32, 0.56, 1.0, 1.8 and 3.2 mg/L
- Results: growth inhibition 0, 4.9, 12.8, 34.1, 63.3, 89.8 and 93.5%; growth rate reduction 0, 1.0, 2.8, 9.5, 23.6, 61.8 and 76.6%

Test substance	:	CAS 98-11-3 (benzenesulphonic acid), purity 99.8%.
Conclusion	:	The EC50 for cell growth inhibition was 70 mg/l. The EC50 for growth rate reduction was 73 mg/l.
Reliability	:	(1) valid without restriction - The effects are most probably related to the acidity of the test substance. - The pH of the test solutions at 0, 4.6, 10, 22 and 46 mg/L deviated more than 1 unit due to high algal growth rate.

08.06.2005 (15)

Species	:	other algae: green algae
Endpoint	:	
Exposure period	:	96 hour(s)
Unit	:	g/l
EC50	:	= 502
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	

Test substance	:	CAS 98-11-3 (benzenesulphonic acid).
Reliability	:	(4) not assignable

07.07.2003 (3)

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	:	= 1100 mg/kg bw
Species	:	rat
Strain	:	other: Carworth-Wistar
Sex	:	male
Number of animals	:	5
Vehicle	:	
Doses	:	
Method	:	other: not indicated
Year	:	1962
GLP	:	no
Test substance	:	

Method :

TEST ANIMALS
- Source: in-house colony
- Age: 4-5 weeks
- Number: 5/dose
- Weight at study initiation: 90-120 g

ADMINISTRATION
- Doses: a logarithmic series of single doses was used differing by a factor of two
- Concentration administered: undiluted

EXAMINATIONS: mortality during an observation period of 14 days

STATISTICAL METHOD: method of Thompson using the Tables of Weil

Result : MORTALITY
- Number of deaths at each dose: not indicated (only LD50 is reported)

Test substance : CAS 98-11-3 (benzenesulphonic acid), purity not indicated.

Conclusion : The LD50 is 0.89 (0.36-3.21 ml/kg bw), which is equivalent to 1104 mg/kg bw (d = 1.24 g/cm3).

Reliability : (2) valid with restrictions
Doses used and mortality data are not reported.

07.07.2003 (16)

5.1.2 ACUTE INHALATION TOXICITY

Type	:	other
Value	:	
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	6
Vehicle	:	
Doses	:	concentrated vapour
Exposure time	:	
Method	:	other: not indicated
Year	:	1962
GLP	:	no
Test substance	:	

Method	:	TEST ANIMALS - Number of animals: 6 males or females ADMINISTRATION Exposure to concentrated vapour is continued for time periods in a logarithmic series with a ratio of two extending from 1/4 to 8 hours, until the inhalation period killing about half the number of rats within 14 days of observation period is defined. - Type or preparation of test condition: For exposures of 10, 5 or 2 minutes a static technique was used by saturating the air with 50-100 g of test substance for 24 hours in a closed chamber. For longer periods a flowstream of saturated vapour was used. EXAMINATIONS: mortality
Result	:	Rats exposed for 8 hours: half the number of rats were killed within 14 days.
Test substance	:	CAS 98-11-3 (benzenesulphonic acid), purity not indicated.
Reliability	:	(3) invalid No guideline study. Amount of test substance that the animals were exposed to is not known.

04.06.2003 (16)

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

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Ames test
System of testing	:	TA97, TA98, TA100 and TA1535
Test concentration	:	0, 100, 333, 1000, 3333, 6667 (without activation) and 10000 (with activation) µg/plate
Cytotoxic concentr.	:	> 10000 µg/plate
Metabolic activation	:	with and without
Result	:	negative
Method	:	other: not indicated
Year	:	1988
GLP	:	no data
Test substance	:	
Method	:	TEST SYSTEM - Species/cell type: TA97, TA98, TA100 and TA1535

- Deficiency: histidine
- Metabolic activation system: liver S9 fraction (Aroclor 1254-induced) from rats (10 and 30%) and hamsters (10 and 30%)

ADMINISTRATION
- Dosing: 0, 100, 333, 1000, 3333, 6667 (without activation) and 10000 (with activation) µg/plate
- Number of replicates: 3
- Application: preincubation assay
- Positive controls: 2-aminoanthracene (all strains with S9); 4-nitro-o-phenylenediamine (TA98 without S9); sodium azide (TA100 and TA1535 without S9); 9-aminoacridine (TA97 without S9)
- Negative control: DMSO
- Pre-incubation time: 20 min

CRITERIA FOR EVALUATING RESULTS
- Statistical method: Margolin (1981) if result is positive

Result : GENOTOXIC EFFECTS
- With metabolic activation (rat): negative
- With metabolic activation (hamster): negative
- Without metabolic activation: negative

PRECIPITATION CONCENTRATION: 10000 µg/L

CYTOTOXIC CONCENTRATION
- With metabolic activation: >10000 µg/L
- Without metabolic activation: >10000 µg/L

Test substance : CAS 98-11-3 (benzenesulphonic acid), purity >=97%.

Reliability : (2) valid with restrictions
Peer-reviewed, standard article.

09.05.2003 (17)

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

(1) SAX's Dangerous Properties of Industrial Materials, (Ed. R.J. Lewis Sr., 9th Ed., Van Nostrand Reinhold, NY, 1996, p. 340.

(2) Merck Index, CD-rom 2000.

(3) EPISuite v.3.10, April 2001.

(4) Lindner, O., Ullmann's Encyclopedia of Industrial Chemistry, Ed. W. Gerhartz, 5th Ed., VCH Verlag, A3, 1985, p.515, 517-518.

(5) NOTOX BV, Calculation of the vapour pressure of benzenesulphonic acid, Project 408847, 2004

(6) Pallas 2.1, 1994/95.

(7) Alonso MC; Pocurull E; Marce RM; Borrull F; Barcelo D; Monitoring of aromatic monosulfonic acids in coastal waters by ion-pair liquid chromatography followed by electrospray-mass spectrometric detection; Environmental Toxicology and Chemistry 21(10): 2059-2066, 2002.

(8) Pitter, P., Determination of biological degradability of organic substances, Water Res. 10: 231-235, 1976.

(9) Alexander, M; Lustigman, BK; Effect of chemical structure on microbial degradation of substituted benzenes; J. Agric. J. Food Chem. 14: 410-3, 1966.

(10) Kawasaki, M.; Experiences with the test scheme under the chemical control law of Japan: an approach to structure-activity correlations; Ecotoxic. Environ. Safety 4: 444-54, 1980.

(11) Kuhn, EP; Suflita, JM; Anaerobic biodegradation of nitrogen-substituted and sulfonated benzene aquifer contaminants; Waste Hazard. Mater. 6 (2): 121-33, 1989.

(12) Kawahara K(a); Yakabe Y; Ohide T; Kida K; Evaluation of laboratory-made sludge for an anaerobic biodegradability test and its use for assessment of 13 chemicals; Chemosphere 39(12): 2007-2018, 1999.

(13) Thurnherr, T; Köhler, T; Cook, AM; Leisinger, T; Microbial degradation of benzenesulfonic acid and its derivatives; 44th Annual meeting of the Schweizerische Gesellschaft fuer Mikrobiologie (Swiss Soc. of Microbiology), Geneva, Switzerland, Apr. 11-13, 1985. Experientia (Basel): 42(1) 1986. 96.

(14) NOTOX BV, Acute toxicity study in Daphnia Magna with Benzenesulfonic acid (static), Project 418725, 2005

(15) NOTOX BV, Fresh water algal growth inhibition test with Benzenesulfonic acid, Project 418736, 2005

(16) Smythe, HF; Carpenter, CP; Weil, CS; Pozzani, UC; Striegel, JA; American Ind. Hygiene Association Journal 23: 95-107, 1962.

(17) Zeiger, E; Anderson, B; Haworth, S; Lawlor, T; Mortelmans, K; Speck, W; Salmonella mutagenicity tests: III. Results from the testing of 255 chemicals, Environmental Mutagenesis 9 (Suppl.9): 1-110, 1988.