201-15302

Appendix

I U C L I D

Data Set

Existing Chemical	:	ID: 1333-39-7
CAS No.	:	1333-39-7
EINECS Name	:	hydroxybenzenesulphonic acid
EC No.	:	215-587-0
TSCA Name	:	Benzenesulfonic acid, hydroxy-
Molecular Formula	:	C6H6O4S

Producer related part

Company	:	Notox
Creation date	:	14.04.2003

Substance related part

Company	:	Notox
Creation date	:	14.04.2003
Status	:	
Memo	:	
Printing date	:	22.04.2004
Revision date	:	
Date of last update	:	19.04.2004
Number of pages	:	15
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	:	= 129 °C
Sublimation	:	
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	
Remark	:	For comparison: * 2-hydroxybenzenesulphonic acid (CAS 609-46-1) decomposes at 145 deg C (Lide, DR (ed.); CRC Handbook of Chemistry and Physics; 80th Ed., 1999-2000, CRC Press LLC, Boca Raton, FL). * 4-hydroxybenzenesulphonic acid (with 1 mol water; CAS 98-67-9) has a melting point of 138-142 deg C (Beilstein Online database).
Test substance	:	CAS 1333-39-7 (hydroxybenzenesulphonic acid).
Reliability	:	(2) valid with restrictions

28.04.2003 (1)

2.2 BOILING POINT

Value	:	= 270 °C at
Decomposition	:	
Method	:	other: estimated
Year	:	1995
GLP	:	
Test substance	:	
Remark	:	Boiling point is 518 °F. For comparison: Benzenesulphonic acid has a boiling point of 171-172 deg C at 0.13 hPa. (Lindner O. 1985; Ullmann's Encyclopedia of Industrial Chemistry. 5th Ed., A3: 515, 517-518 (1985); W. Gerhartz, Ed. VCH Verlag). Using NOMO5 (Mitre Corporation, Version 2.0, 12/4/87), this boiling point is estimated to be 404 deg C at atmospheric pressure.
Test substance	:	CAS 1333-39-7 (hydroxybenzenesulphonic acid), 65% in water.
Reliability	:	(4) not assignable

19.04.2004 (2) (3)

2.3 DENSITY

Type	:	relative density
Value	:	ca. 1.35 at 25 °C
Method	:	other: estimated
Year	:	2002
GLP	:	
Test substance	:	
Test substance	:	CAS 1333-39-7 (hydroxybenzenesulphonic acid), purity not indicated.
Reliability	:	(4) not assignable

19.04.2004 (3)

Type	:	relative density
Value	:	= 1.33 - 1.375 at °C

Test substance : CAS 1333-39-7 (hydroxybenzenesulphonic acid), 65% in water.
Reliability : (4) not assignable
15.04.2003 (2)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : = .00000044 at 25 °C
Decomposition :
Method : other (calculated)
Year :
GLP :
Test substance :

Test substance : CAS 1333-39-7 (hydroxybenzenesulphonic acid).
Reliability : (2) valid with restrictions
28.04.2003 (1)

2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water
Log pow : = -1.65 at °C
pH value :
Method : other (calculated)
Year :
GLP :
Test substance :

Test substance : CAS 1333-39-7 (hydroxybenzenesulphonic acid).
Reliability : (2) valid with restrictions
15.04.2003 (1)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : = 1000 g/l at 25 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :

Test substance : CAS 1333-39-7 (hydroxybenzenesulphonic acid).
Reliability : (2) valid with restrictions
15.04.2003 (1)

Solubility in : Water
Value : 100 vol% at 25 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :

pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: estimated
Year	:	
GLP	:	
Test substance	:	

Test substance	:	CAS 1333-39-7 (hydroxybenzenesulphonic acid), 65% in water.
Reliability	:	(4) not assignable

19.04.2004 (2) (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	:	pKa calculated
Remark	:	The pKa was calculated to be -2.19 for the sulphonate group and 9.05 for the hydroxyl group.
Reliability	:	(2) valid with restrictions

15.04.2003 (4)

3.1.1 PHOTODEGRADATION

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

Remark :

AOP Program (v1.90) Results:
==========
SMILES : Oc1ccc(cc1)S(=O)(=O)O
CHEM :
MOL FOR: C6 H6 O4 S1
MOL WT : 174.17
---------- SUMMARY (AOP v1.90): HYDROXYL RADICALS ----------
Hydrogen Abstraction = 0.0000 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.2800 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 = 7.1252 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 7.4052 E-12 cm3/molecule-sec
HALF-LIFE = 1.444 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 17.333 Hrs
..... ** Designates Estimation(s) Using ASSUMED Value(s)
---------- SUMMARY (AOP v1.90): OZONE REACTION ----------

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

NOTE: Reaction with Nitrate Radicals May Be Important!

Test substance	:	CAS 1333-39-7 (hydroxybenzenesulphonic acid).
Reliability	:	(2) valid with restrictions

15.04.2003 (1)

3.1.2 STABILITY IN WATER

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

Remark	:	EXPERT STATEMENT Benzene sulphonic acid does not contain any hydrolysable groups. It only ionizes in water.
Test substance	:	CAS 1333-39-7 (hydroxybenzenesulphonic acid).
Reliability	:	(2) valid with restrictions

22.03.2004

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 :
Molecular Wt: 174.17
Henry's LC : 2.62e-013 atm-m3/mole (Henrywin program)
Vapor Press : 3.33e-007 mm Hg (Mpbpwin program)
Liquid VP : 3.54e-006 mm Hg (super-cooled)
Melting Pt : 129 deg C (Mpbpwin program)
Log Kow : -1.65 (Kowwin program)
Soil Koc : 0.00918 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	3.6e-014	34.7	0
Water	99.8	360	1000
Soil	8.73e-008	360	0
Sediment	0.166	1.44e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.38e-025	2.47e-012	1.23e-012	2.47e-013	1.23e-013
Water	2.57e-018	658	342	65.8	34.2
Soil	8.32e-026	5.76e-007	0	5.76e-008	0
Sediment	2.14e-018	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: 34.66
Water: 360
Soil: 360
Sediment: 1440
Biowin estimate: 3.013 (weeks)

Advection Times (hr):
Air: 100
Water: 1000

Sediment: 5e+004

Test substance : CAS 1333-39-7 (hydroxybenzenesulphonic acid).
Reliability : (2) valid with restrictions
13.08.2003 (1)

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic
Inoculum : activated sludge, adapted
Concentration : 500 mg/l related to Test substance
related to
Contact time : 72 hour(s)
Degradation : (±) % after
Result :
Deg. product :
Method : other: not indicated
Year : 1966
GLP : no
Test substance :

Method : INOCULUM/TEST ORGANISM
- Inoculum: 5000 mg/L in test solution
- Source: sewage treatment plant
- Preparation of inoculum: fill-and-draw unit containing 1.5 L of mixed liquor; air was supplied at a rate to keep the floc in suspension; every 24 hours the air was shut off and the floc allowed to settle; 1 L of supernatant liquor was wasted and was replaced by an equivalent volume of nutrient solution containing glucose (500 mg/L). Then gradually increased amounts of benzene were added over a 20-day period until benzene had reached a concentration of 250 mg/L.
- Pretreatment: benzene-fed (sole source of carbon); the inoculum used is then taken 16 hr after batch feeding and concentrated to 5000 mg/L

TEST SYSTEM
- Preparation of test solution: 10 ml of adapted sludge suspension (5000 mg/L) and 10 ml of test substance solution (1000 mg/L in 2% phosphate buffer (pH 7.0-7.3))
- Initial test substance concentration (mg C/L): 207 mg C/L (500 mg test substance/L)
- Culturing apparatus: Warburg constant-column respirometer with 125-ml flasks
- Number of culture flasks per concentration: not indicated
- Test duration: 72 hours
- Sampling: at about 28, 40, 54 and 72 hours
- Analytical parameter: oxygen consumption
- ThOD: 1.287 mg/mg (= 643.5 mg O2/L)

TEST CONDITIONS
- Composition of mineral solution: 500 mg/L dibasic potassium phosphate, 500 mg/L Calgonite, 325 mg/L ammonium phosphate and 50 mg/L ferric chloride in tap water
- Test temperature: 20 °C

CONTROLS: inoculum only

Result : The oxygen uptake has been graphically depicted. The oxygen uptake is lower for p-phenolsulphonic acid than for the control. The test substance inhibits the microorganisms in the benzene-adapted sludge.

Test substance : other TS: CAS 98-67-9 (p-hydroxybenzenesulphonic acid), purity analytical grade.

Reliability : (4) not assignable
1. The information is limited to the above mentioned.
2. The test is no guideline test. Adapted microorganisms are used. The concentration of the test substance and of the inoculum are higher than in OECD 302C (30 mg/L and 100 mg/L for test substance and inoculum is recommended, respectively).

22.04.2003 (5)

Type : aerobic
Inoculum : other: soil microorganisms
Concentration : 75 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: 31 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 (abiotic control); 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 260 nm relative to soil-medium mixture without chemical

TEST CONDITIONS
- Composition of mineral solution: 1.6 g K_2HPO_4, 0.40 g KH_2PO_4, 0.50 g NH_4NO_3, 0.20 g $MgSO_4.7H_2O$, 25 mg $CaCl_2.2H_2O$, 2.3 mg $FeCl_3.6H_2O$ in 1 L of distilled water
- Test temperature: 25 °C

Result : The time necessary for complete degradation was established to be 32 days. The degradation was due to biological activity, because no decreased absorbance was seen in vessels with $HgCl_2$.

Test substance : other TS: CAS 98-67-9 (p-hydroxybenzenesulphonic acid), purity not indicated.

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

28.04.2003 (6)

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 275 nm. Results: Sulphate-reducing slurry (0, 13 months): 188, 198 µM Methanogenic slurry (0, 13 months): 194, 235 µM
Test substance	:	other TS: CAS 98-67-9 (p-hydroxybenzenesulphonic acid), purity not indicated.
Conclusion	:	No biodegradation was observed for p-hydroxybenzenesulphonic acid.
Reliability	:	(4) not assignable

22.04.2003 (7)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	
Species	:	
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	= 45329
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	

Remark	:	Value calculated for ECOSAR class phenol-acid.
Test substance	:	CAS 1333-39-7 (hydroxybenzenesulphonic acid).
Reliability	:	(4) not assignable

28.04.2003 (1)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
EC50	:	= 2916
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	

Remark	:	Value calculated for ECOSAR class phenol-acid.
Test substance	:	CAS 1333-39-7 (hydroxybenzenesulphonic acid).
Reliability	:	(4) not assignable

28.04.2003 (1)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	other algae: green algae
Endpoint	:	
Exposure period	:	96 hour(s)
Unit	:	g/l
EC50	:	= 1500
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	

Remark	:	Value calculated for ECOSAR class phenol-acid.
Test substance	:	CAS 1333-39-7 (hydroxybenzenesulphonic acid).
Reliability	:	(4) not assignable

28.04.2003 (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	:	= 1900 mg/kg bw
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	
Year	:	1973
GLP	:	
Test substance	:	
Remark	:	Mean value of males and females. The information given was limited to the above mentioned.
Test substance	:	CAS 1333-39-7 (hydroxybenzenesulphonic acid), purity not indicated.
Reliability	:	(4) not assignable

15.03.2004 (8) (9)

Type	:	LD50
Value	:	= 1500 mg/kg bw
Species	:	mouse
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	
Year	:	1973
GLP	:	
Test substance	:	
Remark	:	Mean value of males and females is 1525 mg/kg.
Test substance	:	CAS 1333-39-7 (hydroxybenzenesulphonic acid), purity not indicated.
Reliability	:	(4) not assignable

03.06.2003 (8) (9)

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

Species	:	rabbit
Concentration	:	
Dose	:	.1 ml
Exposure time	:	
Comment	:	
Number of animals	:	9
Vehicle	:	
Result	:	corrosive
Classification	:	
Method	:	other: not indicated
Year	:	1962
GLP	:	no
Test substance	:	

Method :

TEST ANIMALS
- Number of animals: 3 animals/exposure time

ADMINISTRATION/EXPOSURE
- Amount of substance instilled: 0.1 ml
- Exposure time: 5, 10 or 30 seconds (eyes were rinsed with isotonic saline)

EXAMINATIONS
- Scoring system: Draize, Woodard and Calvery
- Observation times: 1, 4, 24, 48, 72, 120 and 168 hours after exposure

Result :

AVERAGE SCORE (24, 48 and 72 hours)
- Overall irritation score for 5 seconds: 83.6 out of 110
- Overall irritation score for 10 seconds: 110 out of 110
- Overall irritation score for 30 seconds: 110 out of 110

DESCRIPTION OF LESIONS:
5 seconds:
Copious discharge, swelling with the lids about half closed, severe redness of the conjunctivae, and opacity sufficient to render the iris invisible developed within a few minutes. After 14 days there is moderate edema and discharge, moderately severe erythema, and opalescent areas. The iris is reacting to light.

10 seconds:
Same as for 5 seconds and the iris seems to be destroyed after 14 days. Maximum score of 110 already reached after 4 hours.

30 seconds: Severe edema and congestion extending for a considerable distance around the eye displayed rapidly after exposure. Iris is still invisible after 14 days and seems to be destroyed. Maximum score of 110 already reached after 4 hours.

REVERSIBILITY: not within 14 days

OTHER EFFECTS: The animals jumped immediately upon application and the cornea became opalescent in 4-8 seconds. There was rapid swelling in all instances.

Test substance : CAS 1333-39-7 (hydroxybenzenesulphonic acid), 65%.

Reliability : (2) valid with restrictions
The information given is limited to the above mentioned.

23.03.2004 (10)

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

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

9. References

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

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