201-14744B

# Appendix



# IUCLID

# 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** | : | 12.09.2003 |
| **Revision date** | : | |
| **Date of last update** | : | 13.08.2003 |
| **Number of pages** | : | 14 |
| **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 |

### 2.1 MELTING POINT

| | | |
|---|---|---|
| **Value** | : | = 129 °C |
| **Sublimation** | : | |
| **Method** | : | other: calculated |
| **Year** | : | |
| **GLP** | : | |
| **Test substance** | : | |
| **Test substance** | : | CAS 1333-39-7 (hydroxybenzenesulphonic acid). |
| **Reliability** | : | (2) valid with restrictions |
| 28.04.2003 | | (1) |

### 2.2 BOILING POINT

| | | |
|---|---|---|
| **Value** | : | = 270 °C at |
| **Remark** | : | Boiling point is 518 °F. |
| **Test substance** | : | CAS 1333-39-7 (hydroxybenzenesulphonic acid), 65% in water. |
| **Reliability** | : | (4) not assignable |
| 22.04.2003 | | (2) (3) |

### 2.3 DENSITY

| | | |
|---|---|---|
| **Type** | : | relative density |
| **Value** | : | ca. 1.35 at 25 °C |
| **Test substance** | : | CAS 1333-39-7 (hydroxybenzenesulphonic acid), purity not indicated. |
| **Reliability** | : | (4) not assignable |
| 22.04.2003 | | (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** :

**Test substance** : CAS 1333-39-7 (hydroxybenzenesulphonic acid), 65% in water.
**Reliability** : (4) not assignable
22.04.2003 (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

### 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<br>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 + $HgCl_2$ (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. |
| **Test substance** | : | CAS 1333-39-7 (hydroxybenzenesulphonic acid), purity not indicated. |
| **Reliability** | : | (4) not assignable |

03.06.2003 (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

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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