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HPV Assessment Report
On
Hydroxybenzenesulphonic acid
CAS No. 1333-39-7

September 12, 2003

Submitted on behalf of the Aromatic Sulfonic Acids Association
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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) Challenge Program for hydroxybenzenesulphonic acid, (CAS 1333-39-7). Hydroxybenzenesulphonic acid is one of several sulphonic acid based industrial chemicals used as a chemical intermediate and a resin binding catalyst. The substance is classified as a high production volume (HPV) chemical according to criteria 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 hydroxybenzenesulphonic acid (CAS 1333-39-7). No data were available from sponsors. For the development of screening health and environmental assessment information, NOTOX examined the public literature. A literature search performed in March 2003 did not yield any additional results to the existing data in the ECB IUCLID. Then the suitability of studies retrieved on hydroxybenzenesulphonic acid for meeting the SIDS data requirements was determined (summarised in chapter 2), a SIDS data matrix was constructed and recommendations for the draft testing scheme were formulated (data availability analysis; chapter 3). Robust summaries are presented in separate documents as IUCLID data sets.

2. Evaluation of SIDS endpoints

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

The substance under consideration is a sulphonic acid. Hydroxybenzenesulphonic acid is very acidic and in watery environments it is almost completely ionised, even at low pH. The substance is sold as a commercial preparation of 60-70% in water and contains less than 2% phenol and less than 3% sulphuric acid.

2.1. Physico-chemical endpoints

Adequate data on melting point, boiling point, relative density and vapour pressure all are available. The measured value for water solubility is confirmed by the calculated value. The partition coefficient was calculated to be very low as expected from the structural formula; the substance dissolves to a much larger extent in water than in octanol. The dissociation constant for the sulphonic acid group as well as for the hydroxyl group were calculated to be –2.19 and 9.05. This means that the sulphonic acid will be primarily ionised in water.

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

Hydroxybenzenesulphonic acid CAS 1333-39-7				
	Value	**Comment**	**KL.**	**Ref**
Melting point (°C)	129	calculated	2	3
Boiling point (°C)	270	MSDS	4	1,2
Relative Density	1.35	MSDS	4	1,2
Vapor pressure (hPa)	4.4E-07	calculated	2	3
Partition coefficient (log K_{ow})	-1.65	calculated	2	3
Water solubility (g/L)	100 vol%		4	1,2
	1000	calculated	2	3
Dissociation constant (pKa)	-2.19/9.05	calculated	2	4

Kl. = Klimisch criteria
Ref = Reference number

2.2. Environmental fate

The half-life for reaction of hydroxybenzenesulphonic acid with hydroxyl radicals in the atmosphere was estimated to be 17.3 hours. No hydrolysable groups are present in hydroxybenzenesulphonic acid. Distribution in the environment was calculated at Mackay Level III. If the sulphonic acid is released to the environment it will be to the water compartment and stay there (see table below)..
For biodegradability no data are available. From non-standard tests available on p-hydroxybenzenesulphonic acid (one of the components of hydroxybenzenesulphonic acid) it seems likely that hydroxybenzenesulphonic acid is not readily biodegradable. This is confirmed by the calculated probability for MITI linear biodegradation by EPISuite (0.3 = not readily biodegradable). To confirm that hydroxybenzenesulphonic acid is biodegradable an inherently biodegradability test is recommended.

Conclusion: For all relevant endpoints on environmental fate, data are available, except for biodegradation. Therefore, a biodegradation study testing inherent biodegradation has to be

performed.

Hydroxybenzenesulphonic acid CAS 1333-39-7				
	Value	Comment	KL.	Ref
Photodegradation (t1/2)	17.3 hours		2	3
Hydrolysis (t1/2)	-			
Distribution in water/air/soil/sediment	99.8/0. /0.0/0.17%	calculated (emission to water only)	2	3
Biodegradability	-			

Kl. = Klimisch criteria
Ref = Reference number

2.3. Ecotoxicity

For ecotoxicity no measured data are available. Calculation of the relevant endpoints with the ECOSAR model predicts that hydroxybenzenesulphonic acid is not toxic for aquatic species.

Conclusion: Two of the species should be tested. If the resulting measured data are in agreement with the calculated data no further testing is warranted; if the resulting measured data disagree with the calculated data also the third species has to be tested.

Hydroxybenzenesulphonic acid CAS 1333-39-7				
	Value	Comment	KL.	Ref
Acute fish (96-h LC50, mg/L)	45329	calculated	4	3
Acute invertebrates (48-h EC50, mg/L)	2916	calculated	4	3
Algal inhibition (96-h EC50, mg/L)	1.5E06	calculated	4	3

Kl. = Klimisch criteria
Ref = Reference number

2.4. Mammalian toxicity

2.4.1. Acute toxicity

Two oral route values for rat and mouse are available of 1900 and 1500 mg/kg bw, respectively. Since these values are similar, no further testing is considered necessary.

2.4.2. Genetic toxicity

No data are available, so an Ames test and a chromosomal aberration study are warranted.

2.4.3. Repeated dose toxicity

No data are available, so repeated dose toxicity can be considered a data gap. A 28-day repeated dose study must be performed.

2.4.4. Repro/developmental toxicity

No data are available on this endpoint, so a repro/developmental study should be performed.

Conclusion mammalian toxicity: Acute toxicity has been sufficiently investigated. For genetic toxicity an Ames test and a chromosomal aberration test need to be performed. Repeated dose toxicity needs to be covered with a 28-day study. Repro/developmental toxicity needs to be investigated. Based on the data available this can most appropriately be executed in a combined study with repeated dose toxicity (OECD422).

Hydroxybenzenesulphonic acid CAS 1333-39-7				
	Value	**Species**	**KL.**	**Ref**
Acute toxicity				
Acute oral (LD50, mg/kg)	1900	rat	4	8, 9
	1500	mouse	4	
Acute dermal (LD50, mg/kg)	-			
Acute inhalation (LC50, mg/m^3)	-			
Genetic toxicity				
in vitro gene mutation (Ames test)	-			
Chromosomal aberration	-			
Repeated dose	-			
Repro/developmental toxicity	-			

Kl. = Klimisch criteria
Ref = Reference number

2.5. Data availability matrix

Summary of the available data for all SIDS endpoints.

Hydroxybenzenesulphonic acid CAS 1333-39-7				
	Value	**Comment/Species**	**KL.**	**Ref**
Physicochemical properties				
Melting point (°C)	129	calculated	2	3
Boiling point (°C)	270	MSDS	4	1,2
Density (g/cm^3)	1.35	MSDS	4	1,2
Vapor pressure (hPa)	4.4E-07	calculated	2	3
Partition coefficient (log K_{ow})	-1.65	calculated	2	3
	100 vol%		4	1,2
Water solubility (mg/L)	1000	calculated	2	3
Dissociation constant (pKa)	-2.19/9.05		2	4
Environmental fate				
Photodegradation (t1/2)	17.3 hours		2	3
Hydrolysis (t1/2)	-			
Distribution in water/air/soil/sediment	99.8/0./0.0/0.17 %	calculated (emission to water only)	2	3
Ready biodegradability	-			
Ecotoxicity				
Acute fish (96-h LC50, mg/L)	45329	calculated	4	3
Acute invertebrates (96-h EC50, mg/L)	2916	calculated	4	3
Algal inhibition (EC50, mg/L)	1.5E06	calculated	4	3
Mammalian toxicity				
Acute toxicity				
Acute oral (LD50, mg/kg)	1900	rat	4	8,9
	1500	mouse	4	

Hydroxybenzenesulphonic acid CAS 1333-39-7				
	Value	**Comment/Species**	**KL.**	**Ref**
Acute dermal (LD50, mg/kg)	-			
Acute inhalation (LC50, mg/m^3)	-			
Genetic toxicity				
in vitro gene mutation (Ames test)	-			
Chromosomal aberration	-			
Repeated dose	-			
Repro/developmental toxicity	-			

Kl. = Klimisch criteria
Ref = Reference number

3. Data availability and testing proposal

The availability of data is depicted in the following table. The study that should be performed to fill a data gap has been indicated.

	Hydroxybenzenesulphonic acid CAS 1333-39-7
Physico-chemical	
Melting point	+
Boiling point	+
Density	+
Vapor Pressure	+
Partition Coefficient	+
Water Solubility	+
Environmental Fate	
Photodegradation	+
Hydrolysis	+
Distribution in compartments	+
Biodegradability	OECD302
Ecotoxicity*	
96-h LC50 Fish	OECD203
48-h EC50 Daphnia	OECD202
72-h EC50 Algal Inhibition	OECD201
Mammalian toxicity	
Acute	+
Repeated dose	OECD422
Genetic Toxicity	OECD471 + OECD 473
Reproduction/developmental	OECD422

* two out of three should be tested
+ = data available
OECD = test to be performed

Adequate physicochemical data are available. For environmental fate only biodegradability has to be tested. For ecotoxicity two of the species have to be investigated. For mammalian toxicity a combined test for repeated dose toxicity and reproduction/developmental toxicity is warranted. Genetic toxicity should be investigated with a standard Ames test and chromosomal aberration study.

4. References

(1) Dynachem, Inc., MSDS 01/30/95.

(2) Rütgers Organics Corp., MSDS 12/18/02.

(3) EPISuite v.3.10, April 2001.

(4) Pallas 2.1, 1994/95.

(5) Malaney, GW; McKinney, RE; Oxidative abilities of benzene-acclimated activated sludge; Water Sewage Works 113: 302-9, 1966.

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

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

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(9) Shika Igaku, Odontology 36: 317-322, 1973.