TC NES SUBGROUP ON IDENTIFICATION OF PBT AND VPVB SUBSTANCES

RESULTS OF THE EVALUATION OF THE PBT/VPVB PROPERTIES OF:

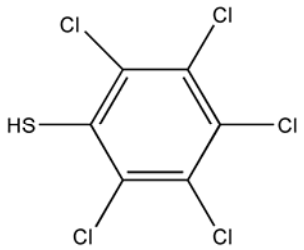
Substance name: Pentachlorobenzenethiol

EC number: 205-107-8

CAS number: 133-49-3

Molecular formula: C6HCl5S

Structural formula:



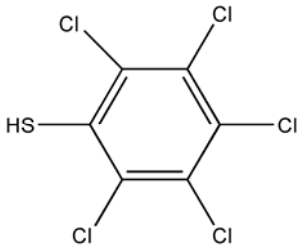
Summary of the evaluation:

Pentachlorobenzenethiol is considered to be a PBT and vPvB substance based on the screening criteria. The substance fulfils the P/vP screening criterion, the vB screening criterion and the T screening criterion. In addition, the substance has a very high potential for long-range atmospheric transport. No further testing is proposed as no producer or importer has been identified.

JUSTIFICATION

1 IDENTIFICATION OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

Name: Pentachlorobenzenethiol
EC Number: 205-107-8
CAS Number: 133-49-3
IUPAC Name:
Molecular Formula: C6HCl5S
Structural Formula:



Molecular Weight: 282.4
Synonyms: Benzenethiol, pentachloro-; Pentachlorothiophenol

1.1 Purity/impurities/additives

No data available.

1.2 Physico-chemical properties

Table 1 Summary of physico-chemical properties

REACH ref Annex, §	Property	Value	Comments
V, 5.1	Physical state at 20 C and 101.3 KPa		
V, 5.2	Melting / freezing point		
V, 5.3	Boiling point		
V, 5.5	Vapour pressure	< 0.022 hPa (at 100ºC) 0.000187 mm Hg (at 2ºC)	Bayer AG data. Study not evaluated. MPBPWIN v1.41
V, 5.7	Water solubility	4.2 mg l^{-1} 0.14 mg l^{-1} (at 25ºC)	Bayer AG data. Study not evaluated. Estimated with WSKOW v1.41
V, 5.8	Partition coefficient n-octanol/water (log value)	6.4 5.91	Bayer AG 1991 (estimated with CLOGP 3.54) Estimated with KOWWIN v1.67
VII, 5.19	Dissociation constant		

2 MANUFACTURE AND USES

According to industry, no production, import or use of pentachlorobenzenethiol occurs at the present in the EU.

3 CLASSIFICATION AND LABELLING

This substance is not classified in the Annex I of Directive 67/548/EEC.

4 ENVIRONMENTAL FATE PROPERTIES

4.1 Degradation (P)

4.1.1 Abiotic degradation

Reaction half-life with OH-radicals in the atmosphere was estimated at 115 days by AopWin v1.91 ($5*10^5$ OH cm^{-3}; 24 h day^{-1}). No estimate for reaction with ozone was provided.

4.1.2 Biotic degradation

A test, according to the OECD 301D (closed bottle test) guideline for ready biodegradability, was conducted in 1979 with a test substance containing approximately 88% pentachlorobenzenethiol. Test concentrations applied were 3, 10 and 30 mg l^{-1} and test duration 30 days. Predominantly domestic sludge was used as inoculum (Bayer AG data as cited in the IUCLID of European Commission, 2000). As 0% degradation was observed, the substance is considered as not readily degradable. It should be noted that the study report was not available to the Rapporteur and the data was therefore not evaluated.

4.1.3 Other information [1]

BIOWIN v4.02 predicts that the substance is not readily biodegradable (MITI models) and that it is recalcitrant according to the ultimate survey models (Biowin3 and Biowin4).

4.1.4 Summary and discussion of persistence

Based on the only available screening test and QSAR-results, pentachlorobenzenethiol is expected to be persistent in the environment.

4.2 Environmental distribution

[1] For example, half life from field studies or monitoring data

4.2.1 Adsorption

Adsorption was not assessed for this substance.

4.2.2 Volatilisation

Pentachlorobenzenethiol is moderately volatile based on its vapour pressure (0.000187 mm Hg = 0.025 Pa). Henry's Law constant is calculated at 50 Pa m^3 mol^{-1} using this vapour pressure and water solubility of 0.14 mg l^{-1}. Hence, the substance is volatile from water.

4.2.3 Long-range environmental transport

Pentachlorobenzenethiol has a high potential for long-range transport via air as it is very slowly degraded in atmosphere. A travelling distance was estimated with ELPOS v1.0.1 at approximately 52,000 km, which is between estimated travelling distances for hexachlorobenzene (CAS 118-74-1) and PCBs. It must be noted, that some uncertainty is embedded in the estimate, because of missing experimental data on physical-chemical properties.

4.3 Bioaccumulation (B)

4.3.1 Screening data[2]

BCFWIN v2.14 resulted a BCF of 7066 (logKow 5.91 applied). BCF of 16,200 was obtained by the Danish (Q)SAR database applying the logBCF 1(Bintein) model.

4.3.2 Measured bioaccumulation data[3]

Measured data on bioaccumulation are not available for the substance.

4.3.3 Other supporting information[4]

No data available.

4.3.4 Summary and discussion of bioaccumulation

QSAR-models predict very high bioaccumulation potential for pentachlorobenzenethiol.

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2 For example, log K_{ow} values, predicted BCFs

3 For example, fish bioconcentration factor

4For example, measured concentrations in biota

5 HUMAN HEALTH HAZARD ASSESSMENT

Data not reviewed for this report.

6 ENVIRONMENTAL HAZARD ASSESSMENT

6.1 Aquatic compartment (including sediment)

6.1.1 Toxicity test results

It should be noted that due to the volatility of pentachlorobenzenethiol, static tests may underestimate the toxicity especially if open test systems are used and no monitoring of test concentrations has occurred.

6.1.1.1 Fish

Acute toxicity

A test conducted in 1990 using the draft method "UBA Verfahrensvorschlag, Mai 1984, Lethale Wirkung beim Zebrabaerbling *Brachydanio rerio* LC_0, LC_{50}, LC_{100}, 48-96 hours" resulted a LC_{50} (96 hours) of 2.4 mg l^{-1} (Bayer AG data as cited in the IUCLID of European Commission, 2000). Part of the test substance remained undissolved in all test concentrations (test concentrations not known). Therefore the result is likely to be an underestimation of the actual toxicity. The study report was not available to the Rapporteur and the study could not be evaluated.

Effects of pentachlorobenzenethiol on *Leuciscus idus* were tested in 1982 using the method "Bestimmung der akuten Wirkungen von Stoffen auf Fische. Arbeitskreis „Fische" im Arbeitskreis „Detergentien" (15.10.73)". Test concentrations are not known and test substance is a product containing approximately 88% pentachlorobenzenethiol. LC_{50} (48 hours) at 0.32 mg l^{-1} was extrapolated using the reported LC_0 of 0.1 mg l^{-1} and LC_{100} of 1 mg l^{-1} (Bayer AG data as cited in the IUCLID of European Commission, 2000). Impurities may have influenced the result. The study report was not available to the Rapporteur and the study could not be evaluated.

Ecosar v0.99h applies the QSAR of phenols to pentachlorobenzenethiol and estimates for fish LC_{50} (96 hours) of 0.162 mg l^{-1}. The Bintein-model applied by the Danish (Q)SAR database determines a LC_{50} of 0.26 mg l^{-1}.

Long-term toxicity

No data available.

6.1.1.2 Aquatic invertebrates

Acute toxicity

The draft test guideline „UBA Verfahrensvorschlag 1994, Bestimmung der Schwimmunfähigkeit beim Wasserfloh *Daphnia magna*. EC_0, EC_{50}, EC_{100} 24 hours, statisches System" was applied in 1990 for testing pentachlorobenzenethiol. EC_{50} (24 hours) at 7.9 mg l^{-1} was determined (Bayer AG data as cited in the IUCLID of European Commission, 2000). The study report was not available to the Rapporteur, and the study could not be evaluated.

Ecosar v0.99h estimates an EC_{50}(48 hours) at 0.382 mg l^{-1} for *Daphnia magna*.

Long-term toxicity

No data available.

6.1.1.3 Algae and aquatic plants

Ecosar v0.99h predicts an EC_{50} (96 hours) of 0.05 mg l^{-1} for green algae.

6.1.2 Sediment organisms

No data available.

6.1.3 Other aquatic organisms

No data available.

6.2 Terrestrial compartment

No data available.

6.3 Atmospheric compartment

No data available.

7 PBT AND vPvB

7.1 PBT, vPvB assessment

Persistence: according to the QSAR-models and the biodegradability screening test available, pentachlorobenzenethiol is not readily biodegradable. It is noted that the study report was not available for evaluation. The substance is considered to meet the P/vP screening criterion.

Bioaccumulation: QSAR models estimate BCFs > 7,000. The screening criterion for vB is clearly fulfilled.

Toxicity: Test data on fish and invertebrates are available showing $L(E)C_{50}$ > 0.1 mg l^{-1}. However, the study reports were not available for evaluation. According to the preliminary judgement, the test results most likely underestimate the actual ecotoxicity. QSARs available predict algae to be most sensitive species with EC_{50} (96 hours) of 0.042 mg l^{-1}, whereas the predicted $L(E)C_{50}$-values for fish and daphnids are just above 0.1 mg l^{-1}. Pentachlorobenzenethiol is therefore considered fulfilling the T screening criterion.

Other supporting information: pentachlorobenzenethiol has a very high potential for atmospheric long-range transport based on its slow atmospheric degradation rate and long predicted atmospheric travelling distance.

Summary: it is concluded that pentachlorobenzenethiol meets the P/vP screening criterion, the vB screening criterion and the T screening criterion. In addition, it has a very high potential for long-range atmospheric transport. No further testing is proposed as no producer or importer was identified.

INFORMATION ON USE AND EXPOSURE

Data not reviewed for the PBT-assessment.

OTHER INFORMATION

The following document was used as the source information:

European Commission (2000) IUCLID Dataset, pentachlorobenzenthiol, CAS 133-49-3, 12.2.2000.