TC NES SUBGROUP ON IDENTIFICATION OF PBT AND VPVB SUBSTANCES

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

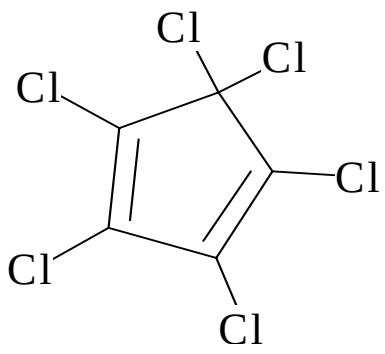
Substance name: Hexachlorocyclopentadiene

EC number: 201-029-3

CAS number: 77-47-4

Molecular formula: C5Cl6

Structural formula:



Summary of the evaluation:

Pure hexachlorocyclopentadiene is not considered to be a PBT substance. It does not fulfil the B criterion, although the screening P criterion and the T criterion are met.

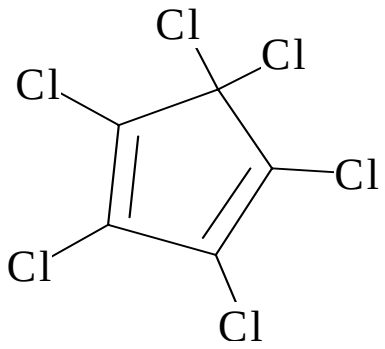
Commercial hexachlorocyclopentadiene may contain hexachlorobuta-1,3-diene; CAS no. 87-68-3, as an impurity. Hexachlorobuta-1,3-diene fulfils the PBT and vPvB criteria. It also fulfils the criteria for new persistent organic pollutants according to the Task Force on POPs to the UNECE's Convention on Long-Range Transboundary Air Pollution. The concentration of this impurity depends on the manufacturing process.

Commercial hexachlorocyclopentadiene may also contain another impurity (hexachlorobenzene; CAS no. 118-74-1). The presence and concentration of this impurity depends on the manufacturing process. Hexachlorobenzene is a persistent organic pollutant (POP) subject to Regulation EC No. 850/2004.

JUSTIFICATION

1 IDENTIFICATION OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

Name: Hexachlorocyclopentadiene
EC Number: 201-029-3
CAS Number: 77-47-4
IUPAC Name:
Molecular Formula: C5Cl6
Structural Formula:



Molecular Weight: 272.77
Synonyms: 1,2,3,4,5,5-hexachlor-1,3-cyclopentadien
1,3-cyclopentadien, 1,2,3,4,5,5-hexachlor
1,3-cyclopentadiene, 1,2,3,4,5,5-hexachloro (8CI, 9CI)
C 56
Graphlox
HCCP
HCCPD
HEX
Hexachloro-1,3-cyclopentadiene
Hexachlorocyclopentadiene
HRS 1655
PCL
Perchlorocyclopentadien

1.1 Purity/Impurities/Additive

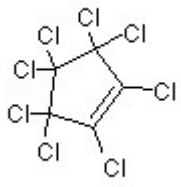
According to European Commission, the only known present producer Velsicol Chemical Corporation at Memphis, Tennessee, USA, provides the substance with a minimum purity of 97 %. The major contaminants found in an industrial preparation of HCCP from Velsicol were octachlorocyclopentene (0.68%), hexachloro-1,3-butadiene (1.11%), tetrachloroethane (0.09%), hexachlorobenzene (0.04%), and pentachlorobenzene (0.02%) (European Commission, 2005).

Information on the actual composition of HCCP and the content of impurities; given by CEFIC to the Norwegian Rapporteur in April 2004 are available:

Hexachlorocyclopentadiene:	99.3 %
Lights (boiling point < 234 ºC):	0.1 %
Hexachlorobutadiene:	0.1 %
Octachlorocyclopentene:	0.3 %
Others (primarily penta- and hexachlorocompounds)	0.2 %

It is noted, that hexachlorobenzene (CAS no. 18-74-1) is a persistent organic pollutant (POP) subject to Regulation EC No. 850/2004. This Regulation defines the relevant concentration limits for substances covered by it.

A PBT assessment for octachlorocyclopentene has been carried out with QSAR as no experimental data are available. According to BioWin (v4.10) the substance is not readily biodegradable. Its predicted log Kow is 4.66 and the predicted BCF is 772 (BCFwin, v2.17). The screening T-criterion is not fulfilled according to Ecosar (v0.99h). Based on QSAR predictions octachlorocyclopentene is therefore not considered to be a potential PBT/vPvB.



Smiles code C1(Cl)=C(Cl)C(Cl)(Cl)C(Cl)(Cl)C1(Cl)(Cl)

Hexachlorobuta-1,3-diene fulfils the PBT and vPvB criteria. Additionally, Hexachlorobuta-1,3-diene fulfils the criteria for new persistent organic pollutants according to the Task Force on POPs of the UNECE's Convention on Long-Range Transboundary Air Pollution. The concentration limits for this substance will be defined under Regulation EC No. 850/2004 after the amendment of the POP Protocol of the UNECE Convention on Long-Range Transboundary Air Pollution has been adopted.

1.2 Physico-Chemical properties

Table 1 Summary of physico-chemical properties. Only values used in the EU risk assessment of HCCP (European Commission, 2005) are presented. For details and references, see European Commission (2005).

REACH ref Annex, §	Property	Value	Comments
VII, 7.1	Physical state at 20 C and 101.3 Kpa	liquid	European Commission (2000)
VII, 7.2	Melting / freezing point	-9°C /-10 °C	Callahan (1979); US Coast guard (1984); Velsicol Chemical Co. (1997)
VII, 7.3	Boiling point	234 °C/239 °C	WHO (1991)
VII, 7.5	Vapour pressure	10 Pa at 25 °C	WHO (1991)
VII, 7.7	Water solubility	1.03-1.25 mg l^{-1} at 22 °C	WHO (1991)
VII, 7.8	Partition coefficient n-octanol/water (log value)	5.04 at 28 °C	Geyer, H. et al. (1984) and Wolfe, N.L. et al. (1982) (measured)
	Dissociation constant	-	

2 MANUFACTURE AND USES

Two producers/importers have provided data under Regulation 93/793/EEC. Currently there are no known producers in the European Union (Silberhorn and Smith, 2001, as cited in European Commission, 2005).

The substance is used in the EU only as intermediate for synthesis of three substances (European Commission, 2005).

3 CLASSIFICATION AND LABELLING

Current classification in the Annex I of Directive 67/548/EEC :

T+; R26 Very toxic by inhalation
T; R24 Toxic in contact with skin
Xn; R22 Harmful if swallowed
C; R34 Causes burns

N; R50-53 Very toxic to aquatic organisms, may cause long term adverse effects in the aquatic environment

4 ENVIRONMENTAL FATE PROPERTIES

4.1 Degradation (P)

4.1.1 Abiotic degradation

Indirect photochemical degradation in the atmosphere is considered to be very slow based on the estimated half-life of 40.8 days for the reaction with OH-radicals using AOP v1.91 (24 h day^{-1}; $5*10^5$ OH^- cm^{-3}). An estimated atmospheric degradation half-life of 29 days was used in the EU risk assessment (European Commission, 2005).

HCCP is expected to undergo hydrolysis. For the EU risk assessment, a hydrolysis half-life of 13.9 days at 12 ºC was used for pH 7 (European Commission, 2005). It is noted, that no information regarding the hydrolysis as a function of pH is available.

Furthermore, a photolysis half-life of 10.7 minutes was applied by European Commission (2005). However, it is noted, that environmentally relevant aquatic exposure occurs in the whole water column and, in the case of HCCP, especially in sediment and soil. Photodegradation of HCCP can be expected to be a relevant removal pathway in the environment only in very shallow clear waters and in the first few centimetres layer of the water column. Therefore aquatic photodegradation is not considered to have relevant impact on the overall persistency of HCCP in the environment.

4.1.2 Biotic degradation

According to the risk assessment (European Commission, 2005) HCCP is considered inherently biodegradable not fulfilling the specific criteria. A biodegradation rate constant of 0 h^{-1} at 12 ºC was applied based on the available data.

BIOWIN v4.02 provides following estimates: BIOWIN2 = 0.00, BIOWIN3 = 1.35 and BIOWIN6 = 0.00.

4.1.3 Other information [1]

In the EU risk assessment, biodegradation studies in soil have been evaluated. Based on the soil studies and biodegradation screening test data, a half-life of 300 days was applied in the risk assessment for soil (European Commission, 2005).

4.1.4 Summary and discussion of persistence

HCCP is considered as inherently biodegradable but not fulfilling the specific criteria. Additionally, BIOWIN–estimates predict that the substance would be persistent in the environment. The available hydrolysis data does not provide an appropriate picture on the hydrolysis rate in the whole environmentally relevant pH–range. HCCP is considered as potentially persistent. Further

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

experimental data, e.g., a full hydrolysis study or degradation simulation tests in water and sediment would be necessary to determine environmentally relevant half-lives.

4.2 Environmental distribution

4.2.1 Adsorption

4.2.2 Volatilisation

4.2.3 Long-range environmental transport

4.3 Bioaccumulation (B)

4.3.1 Screening data

Both the representative logKow of 5.04 and a BCF of 1516 predicted by BCFWIN v2.15 indicate potential for bioaccumulation.

4.3.2 Measured bioaccumulation data

A BCF value for fish of less than 11, representing the steady-state bioconcentration factor of HCCP that was measured in 30-day flow through exposures to constant (measured) levels of HCCP, and a realistic worst case value of 1297 (fish), covering metabolites, have been used in the EU risk assessment (European Commission, 2005). In the available bioaccumulation experiments with fish, HCCP was observed to be metabolised and excreted fast (for details and references, see European Commission, 2005).

4.3.3 Other supporting information[2]

Data not reviewed for this report.

4.3.4 Summary and discussion of bioaccumulation

Despite the logKow of 5.04 HCCP was in several bioaccumulation tests observed to have a low bioaccumulation potential. For the parent compound a BCF < 11 was determined in a reliable flow through test based on measured concentrations, and as the realistic worst case BCF-value 1297 for fish has been identified covering the parent substance and metabolites. It is concluded, that HCCP has a low to moderate bioaccumulation potential.

[2]For 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 Aquatic toxicity test results

Data on acute and long-term aquatic ecotoxicity are available from several studies as evaluated by European Commission (2005). Based on the lowest values of the acute data on freshwater species, fish was observed to be most sensitive followed by invertebrates, whereas algae were least sensitive. For marine species tested, the sensitivity order was for acute ecotoxicity reversed. It is noted, that the lowest ecotoxicity test result for algae is E_rC_{50}(96h) of 3.5 µg l^{-1}(marine species). In the following Table, only the long-term data available (and used for the derivation of PNEC) are presented.

Table 6.1 Long-term aquatic ecotoxicity data used for the PNEC –derivation. For details and references, see European Commission (2005).

Species	Method	Duration	Criterion	Value (µg l^{-1})	Endpoint	Reference
Fish						
Pimephales promelas	FT, M	30 d	NOEC	3.7	Survival	Spehar et al. (1977,1979)
Invertebrates						
Daphnia magna	UBA (1984)	21 d	NOEC	9	Reproduction	Kühn et al. (1989)
Mysidopsis bahia (marine species)	FT, M	28 d	NOEC	0.3	Reproduction	cited in US-EPA (1984)

S = static; FT = flow-through; N = nominal concentrations; M = measured concentrations; NR = not reported.

6.1.2 Sediment organisms

No data available.

6.1.3 Other aquatic organisms

Data not reviewed for this report.

6.2 Terrestrial compartment

Data not reviewed for this report.

6.3 Atmospheric compartment

No data available.

7 PBT AND vPvB ASSESSMENT

Persistence: Hexachlorocyclopentadiene (HCCP) meets the P/vP criteria according to screening data. Based on several available biodegradation screening tests, HCCP is considered as inherently biodegradable but not fulfilling the specific criteria. The substance can also undergo hydrolysis, but it is not possible to judge the relevance of this path over the whole environmentally relevant pH-range. Based on the available experimental data and supported by BIOWIN-estimates, it is considered that HCCP is potentially persistent and further experimental data, e.g., a full hydrolysis study or degradation simulation tests in water and sediment would be necessary to determine environmentally relevant half-lives. However, further testing is not necessary due to the overall conclusion (see below).

Bioaccumulation: HCCP does not meet the B criterion. A BCF < 11 for the parent compound is available from a flow-through test with fish and test substance monitoring. A realistic worst case BCF of 1297 for fish was determined covering the parent substance and the metabolites.

Toxicity: HCCP fulfils the T criterion. The available results from long-term tests have provided a NOEC of 3.7 µg l^{-1} for fish and NOECs of 9 and 0.3 µg l^{-1} for two invertebrate species.

Summary: Pure hexachlorocyclopentadiene does not fulfil the B criterion. The screening P/vP criteria and the T criterion are met. It is concluded that pure hexachlorocyclopentadiene is not considered as a PBT substance.

Commercial hexachlorocyclopentadiene may contain hexachlorobuta-1,3-diene; CAS 87-68-3) , as an impurity. The concentration of this impurity depends on the manufacturing process. Hexachlorobuta-1,3-diene fulfils the PBT and vPvB criteria. Hexachlorobuta-1,3-diene also fulfils the criteria for new persistent organic pollutants according to the Task Force on POPs to the UNECE's Convention on Long-Range Transboundary Air Pollution.

Commercial hexachlorocyclopentadiene may also contain another impurity (hexachlorobenzene; CAS 118-74-1), which is a POP. The presence and concentration of this impurity depends on the manufacturing process. Hexachlorobenzene is a persistent organic pollutant (POP) subject to Regulation EC No. 850/2004.

INFORMATION ON USE AND EXPOSURE

Not relevant as the substance is not identified as a PBT.

OTHER INFORMATION

The information and references used in this report were taken from the following sources:

European Commission, 2005. European Union Risk Assesment Report, Hexachlorocyclopentadiene, CAS No: 77-47-4, Final Draft of December, 2005.

European Commission, 2000. IUCLID Dataset, Hexachlorocyclopentadiene, CAS 77-47-4, 19.2.2000.

Other sources:

CEFIC, 2004. Information on the actual composition of HCCP and the content of impurities