TC NES SUBGROUP ON IDENTIFICATION OF PBT AND VPVB SUBSTANCES

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

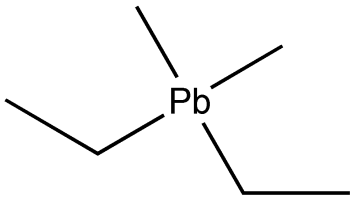
Substance name: Diethyldimethylplumbane

EC number: 217-170-9

CAS number: 1762-27-2

Molecular formula: C6H16Pb

Structural formula:



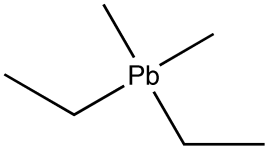
Summary of the evaluation:

Diethyldimethylplumbane is not considered to be a PBT substance. It does not meet the P criterion. The expected degradation products do not fulfil the screening B criterion. The T criterion is fulfilled for the environment and human health. The assessment was mainly based on data of a structurally similar substance, tetraethyl lead (CAS 78-00-2; see PBT Summary No. 91).

JUSTIFICATION

1 IDENTIFICATION OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

Name: Diethyldimethylplumbane
EC Number: 217-170-9
CAS Number: 1762-27-2
IUPAC Name:
Molecular Formula: C6H16Pb
Structural Formula:



Molecular Weight: 295.4
Synonyms: Diethyldimethyllead; ethylmethylplumbane; lead, diethyldimethyl; plumbane, diethyldimethyl; lead alkyl

1.1 PURITY/IMPURITIES/ADDITIVES

No data available.

1.2 PHYSICO-CHEMICAL PROPERTIES

Table 1 Summary of physico-chemical properties. For references, see European Commission (2000)

REACH ref Annex, §	Property	Value	Comments
V, 5.1	Physical state at 20 C and 101.3 Kpa	liquid	European Commission (2000)
V, 5.2	Melting / freezing point		
V, 5.3	Boiling point		
V, 5.5	Vapour pressure	2.9 hPa (at 20ºC)	SDS, The Associated Octel Company Limited (1995) (data not evaluated)
V, 5.7	Water solubility	4.632 mg l^{-1} (at 25ºC; calculated)	WSKOW v1.41 using logKow of 4.04
V, 5.8	Partition coefficient n-octanol/water (log value)	3.9 (calculated) 4.04	KOWWIN v1.67 KOWWIN v1.67 exper. database
VII, 5.19	Dissociation constant		

2 MANUFACTURE AND USES

According to the only former producer, this substance is not produced or imported in the EU at the present. The substance was mainly used as antiknock-agent in gasoline.

3 CLASSIFICATION AND LABELLING

The substance belongs to the group of lead alkyls which are classified according to the 19th and 29th ATP of Directive 67/548/EEC:

Classification

Repr. Cat 1; R61	May cause harm to the unborn child.
Repr. Cat 3; R62	Possible risk of impaired fertility.
T+; R26/27/28	Very toxic by inhalation, in contact with skin and if swallowed.
R33	Danger of cumulative effects
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 fast based on the estimated half-life of 13.7 hours for the reaction with OH-radicals using AOP v1.91 (24 h day^{-1}; $5 \cdot 10^5$ OH^- cm^{-3}). Harrison and Laxen (1978) have observed, that the atmospheric degradation of structurally similar substances tetraethyl lead (CAS 78-00-2) and tetramethyl lead (CAS 75-74-1) in laboratory conditions is dependent on the light intensity. Half-lives in the presence of OH^- and ozone, respectively, were observed to be within few days. It is noted that the data was not evaluated by the Rapporteur.

The rate of hydrolysis was studied by Harrison et al. (1986) according to their own procedure resembling environmentally relevant conditions. A mixture of tetra-alkyl lead compounds (Me_4Pb, $MeEt_3PB$,Me_3Et_3PB, Et_4PB) was used as test substance in concentrations of 3-20 µg l^{-1}. Unfiltered rainwater and filtered (0.45 µm) seawater were used as media. Complete hydrolysis to trialkyl lead compounds occurred in the dark within two days in rainwater and five days in seawater. It must be noted that the report was not available to the Rapporteur for evaluation.

Diethyldimethylplumbane is considered to degrade in a similar manner as tetraethyl lead (CAS 78-00-2; see PBT Summary No. 91) in water:

$$(C_2H_5)_4Pb \rightarrow (C_2H_5)_3Pb^+ \rightarrow (C_2H_5)_2Pb^{2+} \rightarrow [C_2H_5Pb^{3+}] \rightarrow Pb^{2+}$$

Series of degradation steps remove alkyl chains one by one forming as an interim degradation product a corresponding lead alkyl salt. Finally inorganic lead is formed. Inorganic lead is not subject to the PBT -assessment.

Due to a high sorption potential (based on logKow of approximately 4), sediment may be a significant recipient of the substance. No experimental data on degradation of diethyldimethylplumbane in sediment are available. However, such data are considered in the present exposure situation (no production) and due to the expected hydrolysis not necessary.

Further data on degradation of the structurally similar substance have been presented in the PBT Summary No. 91.

4.1.2 Biotic degradation

No standard biodegradation studies are available. BIOWIN v4.02 does not provide consistent predictions for biodegradation:

Linear Model: Biodegrades fast (0.607)
Non-linear Model: Does not biodegrade fast (0.234)
Ultimate Biodegradation: Weeks-months (2.546)
Primary Biodegradation: Days-weeks (3.42)
MITI Linear Model: Not readily biodegrable -(0.0662)
MITI Non-linear Model: Not readily biodegradable (0.0063).

4.1.3 Other information [1]

Extensive monitoring data on the structurally similar substances tetraethyl lead and tetramethyl lead in air, water, sediment, soil and biota are presented by GDCh (1996). The observed lead alkyl concentrations are assumed to be caused largely by emissions from motor vehicle traffic and originate mainly from the 1980s. They are largely very low (in the ng to µg range).

4.1.4 Summary and discussion of persistence

Diethyldimethylplumbane degrades fast in the atmosphere, which is based on vapour pressure and low water solubility expected to be one of the main distribution routes of the substance.

On the basis of the hydrolysis data of Harrison et al. (1986) and reading across from degradation data of the structurally similar substance tetraethyl lead, diethyldimethylplumbane is considered to be not persistent in water. The first degradation products are expected to be trialkyllead salts followed by degradation to dialkyllead salts, alkyllead salts and finally degrading to inorganic lead, which is not subject of this assessment.

Based on the data of tetraethyl lead, diethyldimethylplumbane is expected to be not persistent in soil. Persistency in sediment was not assessed because no data were available. Sediment may be a significant recipient of diethyldimethylplumbane based on its adsorption potential. On the other hand, due to the high volatility, fast atmospheric degradation and hydrolysis in water, sediment is at the present not considered as a relevant compartment of exposure and no further testing is considered necessary.

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

5 ENVIRONMENTAL DISTRIBUTION

Data not reviewed for this report.

5.1.1 Adsorption

5.1.2 Volatilisation

5.1.3 Long-range environmental transport

5.2 BIOACCUMULATION (B)

5.2.1 Screening data[2]

A BCF of 257.5 was predicted by BCFWIN v2.15 using logKow of 4.04.

Triethyllead salt, which is the first hydrolysis product of tetraethyl lead, has a logKow of –1.76 (for details, see PBT Summary No. 91). Similarly, it can be expected that the hydrolysis products of diethyldimethylplumbane (trialkyllead salts) have very low octanol-water partitioning coefficients.

5.2.2 Measured bioaccumulation data[3]

No measured data are available for diethyldimethylplumbane. Bioconcentration data for other tetraalkyl lead compounds are available. For tetraethyl lead experimental BCFs for *Oncorhynchus mykiss* (92-3,189), *Crangon crangon* (20) and *Crassostrea virginica* (18,140) indicate a high bioaccumulation potential. For details of the studies on tetraethyl lead, see PBT Summary No. 91.

BCFs of 2-88 have been obtained for different species in laboratory conditions for triethyllead salt (for details, see PBT Summary No. 91 on tetraethyl lead).

Bioconcentration testing of diethyldimethylplumbane would be necessary to determine its bioaccumulation potential based on the bioaccumulation data of the similar substance tetraethyl lead. Due to the fact that diethyldimethylplumbane is expected to hydrolyse in water, the assessment of bioaccumulation potential of the degradation products would be more relevant for this assessment and testing of the parent compound is not required. Experimental data on triethyl lead salt, which is the hydrolysis product of tetraethyl lead, indicate very low bioaccumulation potential (see PBT Summary No. 91).

5.2.3 Other supporting information[4]

Data not reviewed for this report.

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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

5.2.4 Summary and discussion of bioaccumulation

No experimental data are available on bioaccumulation of diethyldimethylplumbane. Based on read across from data of tetraethyl lead, high bioaccumulation potential cannot be excluded. Further testing would be necessary to determine the bioaccumulation potential. However, it is considered that further testing of diethyldimethylplumbane is not relevant for this assessment. Due to the hydrolysis of the substance, its bioaccumulation in the environment is expected to be negligible.

Assuming similar degradation process as for tetraethyl lead, the first hydrolysis products are expected to be trialkyllead compounds with ethyl and methyl substitutes. Based on the logKow (-1.76) and the experimental BCFs (2-88) of triethyl lead salt, which is the hydrolysis product of tetraethyl lead, it can be expected that the hydrolysis products of diethyldimethylplumbane have a low bioaccumulation potential. Further hydrolysis products (mono- or dialkylated lead salts) are expected to exhibit lower bioaccumulation potential than trialkylated lead salts.

6 HUMAN HEALTH HAZARD ASSESSMENT

Data not reviewed for this report.

7 ENVIRONMENTAL HAZARD ASSESSMENT

7.1 AQUATIC COMPARTMENT (INCLUDING SEDIMENT)

No experimental data are available for diethyldimethylplumbane. For similar substances tetraethyl lead (TEL) and tetramethyl lead (TML), acute ecotoxicity data are available on several fish, invertebrate and algae species. The lowest results are as follows:

LC_{10} (96 hours) = 0.004 mg l^{-1} for *Salmo gairdneri*, TML (Wong et al., 1981).

LC_{50} (96 hours) = 0.05 mg l^{-1} for *Pleuronectes platessa*, TML, closed flow through system (Maddock and Taylor, 1980)

LC_{50} (48 hours) = 0.06 mg l^{-1} for *Morome labrax* larvae, TEL, closed system (Marchetti, 1978)

LC_{50} (96 hours) = 0.02 mg l^{-1} for *Crangon crangon*, TEL, closed flow through system (Maddock and Taylor, 1980)

LC_{50} (48 hours) = 0.08 mg l^{-1} for *Artemia salina*, TEL, closed system (Marchetti, 1978)

EC_{50} (6 hours) = 0.06 mg l^{-1} for *Phaeodactylum tricornutum*, TEL, closed flow through system (Maddock and Taylor, 1980)

It must be noted, that the test reports were not available to the Rapporteur for evaluation. Due to the volatility and degradation of TEL and TML, results from especially static tests without monitoring of test concentration may underestimate their toxicity.

7.1.1 Toxicity test results

7.1.1.1 Fish

Acute toxicity

Long-term toxicity

7.1.1.2 Aquatic invertebrates

Acute toxicity

Long-term toxicity

7.1.1.3 Algae and aquatic plants

7.1.2 Sediment organisms

7.1.3 Other aquatic organisms

7.2 TERRESTRIAL COMPARTMENT

Data not reviewed for this report

7.3 ATMOSPHERIC COMPARTMENT

Data not reviewed for this report.

8 PBT AND VPVB

8.1 PBT, VPVB ASSESSMENT

Persistence: Diethyldimethylplumbane does not fulfil the P criterion. The substance is expected to degrade abiotically in water based mainly on data on the degradation behaviour of the structurally similar substance tetraethyl lead (CAS 78-00-2; see PBT Summary No. 91). The first degradation products are expected to be trialkyllead salts followed by degradation to dialkyllead salts, alkyllead salts and finally degrading to inorganic lead, which is not subject of this assessment.

Persistency in sediment was not assessed, because no data were available. Sediment may be a significant recipient of the substance based on its adsorption potential. On the other hand, due to the volatility, fast atmospheric degradation and hydrolysis in water, sediment is at the present not considered as a relevant compartment of exposure and no further testing is considered necessary.

Bioaccumulation: No bioaccumulation data are available for the parent compound. The bioaccumulation potential of the parent compound may be high based on data on tetraethyl lead but

no further testing is necessary due to the degradation of the substance. The expected degradation products do not meet the screening B criterion.

Toxicity: The substance fulfils the T criterion for the environment and human health based on read across from structurally similar lead compounds. No short- and long-term experimental data are available for diethyldimethylplumbane, but for the structurally similar substances tetraethyl lead and tetramethyl lead short term test data are available. Several $L(E)C_{50}$ –values for invertebrates, fish and algae are considerably below 0.1 mg l^{-1}. Alkyllead compounds are classified as toxic to reproduction in category 1 (R61) and in category 3 (R62), hence fulfilling the T criterion for human health.

Summary: Diethyldimethylplumbane does not meet the P criterion. Based on data from structurally similar alkyl lead compounds it might fulfil the B criterion but its degradation products do not meet the screening B criterion. T criterion is fulfilled for the environment and human health. It is concluded that the substance is not considered as a PBT substance. The assessment was based mainly on data of structurally similar tetraethyl lead (see PBT Summary No. 91).

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 mainly taken from the following source:

European Commission (2000) IUCLID Dataset, diethyldimethylplumbane, CAS 1762-27-2, 18.2.2000.

Other sources:

GDCh (1996) 130 BUA-Report: Tetramethylplumbane CAS-No. 75-74-1; Tetraethylplumbane CAS-No. 78-00-2. Edited by GDCh-Advisory Committee on Existing Chemicals of Environmental Relevance (BUA). ISBN 978-3-7776-0697-2. 386 p.