# TC NES SUBGROUP ON IDENTIFICATION OF PBT AND VPVP SUBSTANCES

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

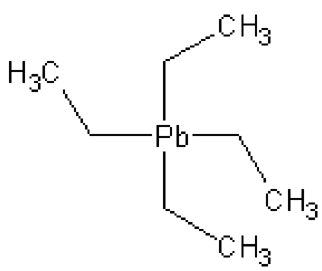
**Substance name: Tetraethyl lead (TEL)**

**EC number: 201-075-4**

**CAS number: 78-00-2**

**Molecular formula: $C_8H_{20}Pb$**

**Structural formula:**




**Summary of the evaluation:**

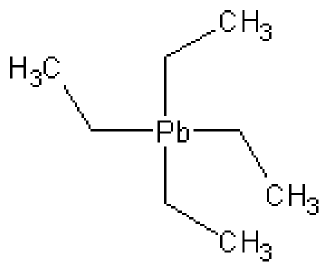
TEL is not considered to be a PBT substance. It does not meet the P criterion and the degradation products do not fulfil the screening B criterion. The T criterion is fulfilled.

The overall conclusion is that both TEL and the main hydrolysis product, triethyl lead salt, should not be listed as PBT substances.

# JUSTIFICATION

## 1 IDENTIFICATION OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

Name: Tetraethyl lead
EC Number: 201-075-4
CAS Number: 78-00-2
IUPAC Name: Tetraethyllead
Molecular Formula: $C_8H_{20}Pb$
Structural Formula:




Molecular Weight: 323.45
Synonyms: TEL, Ethyl plumbane, Lead alkyl, Lead tetraethyl

### 1.1 PURITY/IMPURITIES/ADDITIVES

No information 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 | Liquid | IUCLID (2000) |
| V, 5.2 | Melting / freezing point | -136°C<br>-11.28°C | Exp. database match (EPIWIN)<br>Estimated (EPIWIN v3.12) |
| V, 5.3 | Boiling point | 202°C<br>200.52°C | Exp. database match (EPIWIN)<br>Estimated (EPIWIN v3.12) |
| V, 5.5 | Vapour pressure | 0.35 hPa at 25°C<br>0.63 hPa at 25°C | Exp. database match (EPIWIN)<br>Estimated (EPIWIN v3.12) |
| V, 5.7 | Water solubility | 0.29 mg/l at 26°C<br>2.55 mg/l at 25°C | Exp. database match (EPIWIN)<br>Estimated from log$K_{ow}$ of 4.15 (EPIWIN v3.12) |
| V, 5.8 | Partition coefficient n-octanol/water (log value) | 4.32 at 20°C<br>4.15 (fresh water, pH = 7)<br>4.62 (sea water, pH = 8)<br>4.88 | Measured data (IUCLID, 2000)<br>Exp. database match (EPIWIN)<br>As above<br>Estimated (EPIWIN v3.12) |
| VII, 5.19 | Dissociation constant | | |

## 2 MANUFACTURE AND USES

TEL is produced and used at HPVC tonnage, but is mostly exported from the EU. This substance is yet to complete the UNEP phase-out program on use as a fuel additive for motor engines, and is still used for piston-engine aircrafts and vintage cars.

## 3 CLASSIFICATION AND LABELLING

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

| | |
|---|---|
| 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 of TEL in the atmosphere is considered to be fast based on the estimated half-life of 2.61 hours for the reaction with OH-radicals using EPIWIN v3.12 (24-hour $day^{-1}$; $5*10^5$ $OH^-$ $cm^{-3}$).

Harrison and Laxen (1978) reported rapid decomposition of TEL in the atmosphere predominantly via reaction with OH radicals and ozone. A half-life of 2 days (summer) and 8 days (winter) was estimated.

No standard biodegradation data are available in IUCLID (2000). TEL is not stable in aquatic systems. Dissolved TEL can be either lost by evaporation from the surface water or by stepwise abiotic processes to form lower ethylated lead compounds and ultimately inorganic lead, which is not subject to the PBT-assessment.

Tetraethyl lead is considered to degrade abiotically according to the following sequence:

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

The rate of hydrolysis was studied by Harrison et al. (1986) in a series of experiments designed to replicate environmental conditions using mixtures of tetraalkyl lead compounds ($Me_4Pb$, $MeEt_3Pb$, $Me_3Et_3Pb$, $Et_4Pb$). Unfiltered rainwater and filtered (0.45 µm) seawater were used as media (concentrations of 3-20 µg $l^{-1}$). TEL readily underwent degradation to triethyl lead salt, 50% degradation within 2-5 days depending on the conditions; water purity, sunlight, oxygen content and temperature.

Triethyl lead salts are more stable than TEL in solution, although as with TEL, decomposition reactions are accelerated in sunlight (half-life < 9 days in natural waters) (Blanchard et al., 1984).

Jarvie et al. (1981) reported 90% degradation of TEL in aqueous solution after 15 days.

Due to high sorption potential (based on $logK_{ow}$ of approximately 4), sediment may be a significant recipient of the substance. The limited information available on sediments indicates that TEL undergoes a similar stepwise degradation to form inorganic lead.

Ou at al. (1994) investigated the biological and chemical transformation rate of TEL in surface and sub-surface soils using $^{14}C$ labelled TEL. A 50% reduction in $^{14}C$ TEL concentration occurred within 2 hours in non-sterile soils and within 14 hours in sterile soils. No $^{14}C$ TEL was detected in the soil after 28 days incubation.

Mulroy and Ou (1998) showed that pure TEL is unstable in soils and undergoes complete decomposition to inorganic lead within 14 days.

### 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 (0.5936)

Non-linear Model: Does not biodegrade fast (0.1702)

Ultimate Biodegradation: Weeks-months (2.4844)

Primary Biodegradation: Days-weeks (3.3811)

MITI Linear Model: Not readily biodegradable (-0.0508)

MITI Non-linear Model: Not readily biodegradable (0.0066).

#### 4.1.3 Other information [1]

TEL is a non-polar hydrophobic organic compound. The true solubility of this substance in natural waters (fresh and salt) is around 0.1 mg/l (100 ppm) as lead. TEL has the tendency to form super-saturated solutions, hence the higher solubility values quoted in the literature.

#### 4.1.4 Summary and discussion of persistence

TEL degrades rapidly in the atmosphere. Based on the vapour pressure and low water solubility, atmospheric degradation is expected to be one of the main distribution routes of tetraethyl lead.

Hydrolysis data (Harrison et al., 1986) and available degradation studies indicate that TEL is not persistent in water, decomposing by both biotic and abiotic pathways to form ethyl lead salts (half-life = 2-5 days) and ultimately inorganic lead.

Limited information on sediments indicates that TEL undergoes a similar stepwise degradation in sediment to form inorganic lead. Available data show that TEL is unstable in soils and undergoes complete decomposition within 14 days.

It is concluded that TEL does not meet the P/vP criterion.

### 4.2 ENVIRONMENTAL DISTRIBUTION

#### 4.2.1 Adsorption

#### 4.2.2 Volatilisation

The high value of Henry's Law Constant of $6.9 \times 10^4$ Pa $m^3$ $mol^{-1}$ indicates ready loss of dissolved TEL by volatilization form the surface of water, thus reducing persistence in the environment.

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

## 4.3 BIOACCUMULATION (B)

### 4.3.1 Screening data[2]

A BCF of 313 was predicted for TEL by EPIWIN v3.12 using a log $K_{ow}$ value of 4.15 (from the EPIWIN database). The first hydrolysis product of TEL, triethyl lead has a log $K_{ow}$ value of -1.76.

### 4.3.2 Measured bioaccumulation data[3]

The measured log $K_{ow}$ for TEL is 4.32 (IUCLID 2000). Measured BCF data are reported in IUCLID (2000) for *Crassostrea virginica* (18,140) (Heitmuller and Parrish, 1977), *Crangon crangon* (20) and *Oncorhynchus mykiss* (92-3,189) (Maddock and Taylor, 1980). Most of the BCF values are based on tests with invertebrates (crustaceans and molluscs). It should also be noted that the highest BCF (18,140) for TEL in oysters was recorded from exposure to motor fuel antiknock compound containing 64% TEL and 36% halogenated compounds, which may have affected the accumulation of the TEL component of the mixture. Other marine creatures show much lower BCF factors. The log $K_{ow}$ of TEL is below 4.5. However, overall a high bioaccumulation potential cannot be excluded and the data indicate that TEL may fulfil the B/vB criterion.

However, TEL is not persistent in the environment and hydrolyses in water to lower alkylated lead salts. The main degradation product of TEL, triethyl lead salt has a log $K_{ow}$ of -1.76, which suggests a low potential for bioaccumulation. BCFs of 2-88 have been obtained for different species of fish and shellfish in laboratory conditions for triethyl lead salt (Maddock and Taylor, 1980). Although these laboratory data are old and based on short duration tests (96h), they suggest that the B criterion is unlikely to be met. Triethyl lead is further degraded to di- and monoethyl lead. It can be expected that these hydrolysis products also have low bioaccumulation potential.

### 4.3.3 Other supporting information[4]

Monitoring data in the UK indicate that trialkyl lead salts have the potential to bioaccumulate in shellfish and cause effects in birds that feed on them. There is however considerable uncertainty as to whether these data relate to uptake of triethyl or trimethyl lead.

### 4.3.4 Summary and discussion of bioaccumulation

Based on the measured BCF data for TEL, high bioaccumulation potential cannot be excluded. However, this substance is expected to hydrolyse in water so the assessment of the bioaccumulation potential of the degradation products is relevant. The first hydrolysis products are expected to be triethyl lead salts which have experimental BCFs of 2-88. Triethyl lead salt has a log $K_{ow}$ of -1.76, indicating a low potential for bioaccumulation. This substance is further degraded to di- and monoethyl lead and it can be expected that these hydrolysis products also have low bioaccumulation potential. Thus it is concluded that the degradation products of TEL do not meet the B/vB criterion.

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

3 For example, fish bioconcentration factor

4 For example, measured concentrations in biota

### 4.4 SECONDARY POISONING

## 5 HUMAN HEALTH HAZARD ASSESSMENT

Data are not reviewed for this report.

## 6 ENVIRONMENTAL HAZARD ASSESSMENT

### 6.1 AQUATIC COMPARTMENT (INCLUDING SEDIMENT)

Acute toxicity data are available for several fish, invertebrate and algae species for this substance. The lowest results are as follows:

$LC_{50}$ (96-hour) = 0.06 mg $l^{-1}$ for *Morome labrax* larve, closed system (Marchetti, 1978),

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

$LC_{50}$ (96-hour) = 0.08 mg $l^{-1}$ for *Artemia salima*, closed system (Marchetti, 1978),

$LC_{10}$ (96-hour) = 0.004 mg $l^{-1}$ for *Salmo gairdneri* (Wong et al., 1978),

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

The test reports were not available to the Rapporteur for evaluation and the acute $LC_{50}$ (96-hour) value of 0.02 mg $l^{-1}$ is for a non-standard organism. It should be noted that results without monitoring of test concentrations, particularly static systems, may underestimate the toxicity of TEL due to its volatility and degradation.

On the basis of the available data for TEL, the T-criterion for the environment is considered to be fulfilled.

### 6.2 TERRESTRIAL COMPARTMENT

### 6.3 ATMOSPHERIC COMPARTMENT

### 6.4 INDIRECT EXPOSURE VIA THE FOOD CHAIN

# 7 PBT AND VPVB

## 7.1 PBT, VPVB ASSESSMENT

Persistence: TEL is not persistent in the environment. The substance decomposes by both biotic and abiotic pathways to form ethyl lead salts (half-life = 2-5 days), and ultimately inorganic lead. The main hydrolysis product, triethyl lead salt, is not persistent in the environment and has a half-life in water of less than 15 days. The conclusion is that TEL does not meet the P/vP criteria.

Bioaccumulation: with the exception of one bioaccumulation study with motor fuel antiknock compound rather than pure TEL, available data indicate that the BCF for TEL is < 1;000 and log $K_{ow}$ is < 5. Furthermore, the main hydrolysis product, triethyl lead salt has a very low log $K_{ow}$ of -1.76. BCFs of 2-88 have been obtained for a variety of fish and shellfish species. Di-and monoalkyl lead salt are also expected to have very low bioaccumulation potential. Therefore, the degradation products of TEL are considered not to meet the B/vB criteria.

Toxicity: the substance fulfils the T criterion for the environment. Short term test data are available and several $LC_{50}$ values for invertebrates, fish and algae are considerably below 0.1 mg $l^{-1}$.

Summary: there is strong evidence that TEL does not meet the P/vP criterion due to abiotic and biotic degradation to lower alkylated lead salts and ultimately inorganic lead (not considered further in the PBT assessment). The lower alkylated lead salts are not considered as PBT due to further degradation and probable low bioaccumulation potential. The biodegradation products of TEL do not meet the screening B/vB criterion. It is also concluded that the main hydrolysis product, triethyl lead salt, does not merit classification as a PBT chemical. Although the T criterion is fulfilled, the overall conclusion is that TEL should not be listed as a PBT substance.

# INFORMATION ON USE AND EXPOSURE

Not relevant as substance is not identified as a PBT.

# OTHER INFORMATION

The information used in this report was taken from the following sources:

Blanchard G, Martin G and Charlou J L (1984) International conference of heavy metals in the environment s 1254-1257. Fate and behaviour of TEL in the natural environment.

European Commission (2000) IUCLID Dataset, Tetraethyl lead, CAS 78-00-2, 19.02.2000.

Harrison RM, Hewitt CN and Radojevic (1986) Proc. Int. Con., Chemicals in the environment, Lisbon, s 110-116.

Harrison RM and Laxen DPH (1978) Environ. Sci. Techn., vol 12, pp 1384-1391. Sink processes for tetraalkyl lead compounds in the atmosphere.

Heitmuller T and Parrish R (1977) Report to E. I. DuPont de Nemours from Bionomics Marine Research Laboratory. Bioaccumulation and depuration of lead by eastern oysters exposed to tetraethyl lead motor fuel antiknock compound.

Jarvie AWP, Markell RN and Porter HR (1981) Environmental Res., vol 25, p 241. Decomposition of organolead compounds in aqueous systems.

Maddock BG and Taylor D (1980) Lead in the Marine Environment, Pergammon Press, Oxford, s 2330261. The acute toxicity and bioaccumulation of some alkyl compounds in marine animals.

Marchetti R (1978) Mar. Pollut. Bull., vol. 2, pp. 206-207. Acute toxicity of lead alkyl to some marine organisms.

Mulroy PT and Ou L-T (1998) Environ. Toxicol. Chem., vol 17, pp 777-782. Degradation of tetraethyl lead during the degradation of leaded gasoline hydrocarbons in soil.

Ou L-T, Thomas JE and Jing W (1994) Bull. Environ. Contam. Toxicol., vol 52, pp 238-245. Biological and chemical degradation of tetraethyl lead in soil.

Wong PTS, Chau YK. Kramar O and Bengert GA (1981) Water Res., vol 15, pp 621-625. Accumulation and depuration of tetramethyl lead by Rainbow trout.