

TC NES SUBGROUP ON IDENTIFICATION OF PBT AND VPVB SUBSTANCES

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

Substance name: Hydrocarbons, C4, 1,3-butadiene-free, polymd., dibutylene fraction, hydrogenated

EC number: 297-626-1

CAS number: 93685-78-0

Molecular formula:

Structural formula:

Not applicable.

Summary of the evaluation:

Hydrocarbons, C4, 1,3-butadiene-free, polymd., dibutylene fraction, hydrogenated is not considered to be a PBT substance. It does not meet the B criterion. The screening P/vP criteria are fulfilled. The screening T criterion is not met. The assessment was mainly based on the data of the main component 2,2,4-trimethylpentane (CAS 540-84-1).

JUSTIFICATION

1 IDENTIFICATION OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

Name: Hydrocarbons, C₄, 1,3-butadiene-free, polymd., dibutylene fraction, hydrogenated

EC Number: 297-626-1

CAS Number: 93685-78-0

IUPAC Name:

Molecular Formula: not applicable

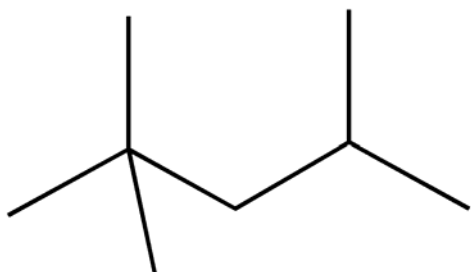
Structural Formula: not applicable

Molecular Weight: not applicable

Synonyms:

1.1 Purity/impurities/additives

According to industry, hydrocarbons, C₄, 1,3-butadiene-free, polymd., dibutylene fraction, hydrogenated is a complex mixture of C₈H_(x-18) saturated hydrocarbons. However, at least 90% of the substance consists of 2,2,4-trimethylpentane (CAS 540-84-1; synonym: isooctane; see structural formula below).



1.2 Physico-chemical properties

Table 1 Summary of physico-chemical properties. For references, see European Commission, 2000a and 2000b

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	50-100 hPa (at 38°C) 53 hPa (at 20°C)	EC Erdölchemie (1993) (data not evaluated) For 2,2,4-trimethylpentane; EC Erdölchemie (1994) (data not evaluated)
V, 5.7	Water solubility	0.1 g l ⁻¹ (at 20°C) 9.91 mg l ⁻¹ (at 25°C) 2.44 mg l ⁻¹ (at 25°C) 2.96 mg l ⁻¹ (at 25°C)	EC Erdölchemie (1994) (data not evaluated) For 2,2,4-trimethylpentane; WSKOW v1.41 using logKow of 4.09 For 2,2,4-trimethylpentane; WSKOW v1.41 exper. database, Yalkowsky and Dannenfelser (1992) For different dimethylhexanes; WSKOW v1.41 using logKow of 4.7
V, 5.8	Partition coefficient n-octanol/water (log value)	4.09-4.53 4.09 (calculated) 4.7	For 2,2,4-trimethylpentane; different estimations; BP Chemicals Ltd. (2003) For 2,2,4-trimethylpentane; KOWWIN v1.67 For different dimethylhexanes; CLOGP v3.3; Bayer AG (1989)
VII, 5.19	Dissociation constant	-	

2 MANUFACTURE AND USES

One company has notified the substance under Regulation 93/793/EEC according to European Commission (2000a).

3 CLASSIFICATION AND LABELLING

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

The main component 2,2,4-trimethylpentane is classified as follows:

F; R11	Highly flammable
Xn; R65	Harmful: may cause lung damage if swallowed
Xi; R38	Irritating to skin
Xi; R67	Vapours may cause drowsiness and dizziness
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 the main component 2,2,4-trimethylpentane (CAS 540-84-1) in the atmosphere is considered to be slow based on the estimated half-life of 3.5 days for the reaction with OH-radicals using AOP v1.91 (24 h day⁻¹; 5*10⁵ OH⁻ cm⁻³).

4.1.2 Biotic degradation

Bayer AG (1986) reports in the IUCLID (European Commission, 2000a) a BOD₅/COD-ratio of < 0.2. No further information was provided on the test and it must be noted that the report was not available to the Rapporteur for evaluation.

BIOWIN v4.02 provides for the main component 2,2,4-trimethylpentane following biodegradation predictions:

BIOWIN 1: Biodegrades fast (0.509)

BIOWIN 2: Does not biodegrade fast (0.417)

BIOWIN 3: Weeks-months (2.73)

BIOWIN 4: Days-weeks (3.53)

BIOWIN 5: Does not biodegrade fast (0.441)

BIOWIN 6: Biodegrades fast (0.513).

Ready biodegradability prediction: not readily biodegradable

4.1.3 Other information ¹

Data not available.

4.1.4 Summary and discussion of persistence

Based on the BOD₅/COD-ratio and the BIOWIN -predictions and considering the absence of standard biodegradation data, the substance is concluded to be not readily biodegradable. Although BIOWIN 3 and BIOWIN 6 would indicate that the substance is not persistent, the experimental data and the overall ready biodegradability prediction of BIOWIN are considered to override BIOWIN 3 and BIOWIN 6 predictions.

4.2 Environmental distribution

Data not reviewed for this report.

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

4.2.1 Adsorption

4.2.2 Volatilisation

4.2.3 Long-range environmental transport

4.3 Bioaccumulation (B)

4.3.1 Screening data²

For 2,2,4-trimethylpentane a BCF of 279.2 and 614 were calculated by BCFWIN v2.15 using logK_{ow} of 4.09 and 4.53, respectively. Using the logK_{ow} of 4.7 for dimethylhexanes, a BCF of 830 is predicted by BCFWIN v2.15 applying the standard equation and no correction factor.

4.3.2 Measured bioaccumulation data³

MITI (1992) has tested the main component 2,2,4-trimethylpentane in a standard flow-through test for 28 days using *Cyprinus carpio*. The test system was designed to take the volatility of the substance into account. BCF range of 440-580 was obtained for test concentration of 10 µg l⁻¹ and a BCF range of 460-650 for test concentration of 1 µg l⁻¹. Mean fat content of the fish was 3.49% at the start and 2.84 at the end of the experiment.

No data was provided on whether steady state was reached or not. In similar tests (conducted with other substances and) reported by MITI, the provided BCF range is the range of measured BCFs of each sampling occasion. Both test concentrations are clearly below the water solubility. In addition, there are no obvious reasons (such as molecule size, very low water solubility, high adsorption, fast degradation) which could cause too high variability of exposure concentrations or slow uptake. The results are considered reliable enough for the purpose of this assessment.

4.3.3 Other supporting information⁴

No data available.

4.3.4 Summary and discussion of bioaccumulation

The main component 2,2,4-trimethylpentane has based on a flow-through fish bioconcentration test of MITI (1992) a BCF range of 440-650. The predicted BCF for the main component ranges between 280 and 614 and for diverse dimethylhexane components a BCF of 839 has been calculated. It can be concluded that the substance has a moderate bioaccumulation potential.

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)

Hydrocarbons, C4, 1,3-butadiene-free, polymd., dibutylene fraction, hydrogenated and its main component 2,2,4-trimethylpentane are volatile substances. The IUCLIDs (European Commission, 2000a,b) contain acute ecotoxicity test results from static tests without test substance monitoring. In addition, the acute toxicity values reported are far beyond water solubility of the substances and results are available only for fish. The test reports were not available to the Rapporteur for evaluation, and it is considered that the results as presented in the IUCLIDs are not reliable enough to make conclusions. ECOSAR v0.99h predicts the following acute values:

Fish: LC_{50} (96 hours) = 0.919 mg l⁻¹

Daphnid: LC_{50} (96 hours) = 1.137 mg l⁻¹

Green algae: EC_{50} (96 hours) = 0.802 mg l⁻¹

6.1.1 Toxicity test results

6.1.1.1 Fish

Acute toxicity

Long-term toxicity

6.1.1.2 Aquatic invertebrates

Acute toxicity

Long-term toxicity

6.1.1.3 Algae and aquatic plants

6.1.2 Sediment organisms

6.1.3 Other aquatic organisms

6.2 Terrestrial compartment

Data not reviewed for this report.

6.3 Atmospheric compartment

Data not reviewed for this report.

7 PBT AND vPvB

7.1 PBT, vPvB assessment

Persistence: Hydrocarbons, C4, 1,3-butadiene-free, polymd., dibutylene fraction, hydrogenated fulfils the P/vP screening criteria based on a BOD5/COD ratio of < 0.2 and on QSAR predictions of its main component 2,2,4-trimethylpentane (CAS 540-84-1). Although BIOWIN 3 and BIOWIN 6 models indicate that the screening P criterion would not be fulfilled, the experimental data and other predictions are considered to override the two models. Further testing is necessary to complete the assessment but not required due to the overall conclusion (see below).

Bioaccumulation: the substance does not meet the B criterion. An experimental BCF of 440-650 was obtained for fish in a flow-through test for the main component 2,2,4-trimethylpentane. QSAR predictions for 2,2,4-trimethylpentane and dimethylhexanes are in agreement with the measured BCF.

Toxicity: experimental data are available for 2,2,4-trimethylpentane but they are considered not reliable for this assessment due to the volatility of the substance. Based on the ECOSAR predictions for 2,2,4-trimethylpentane, screening T criterion is not fulfilled. Further experimental data would be necessary to determine the actual ecotoxicity, but such data are not required due to the overall conclusion of the assessment (see below).

Summary: Hydrocarbons, C4, 1,3-butadiene-free, polymd., dibutylene fraction, hydrogenated does not meet the B criterion based on a measured BCF of 440-650 for its main component 2,2,4-trimethylpentane (CAS 540-84-1). The main component meets the screening P/vP criteria. The screening T criterion is not fulfilled based on QSAR predictions. It is concluded that hydrocarbons, C4, 1,3-butadiene-free, polymd., dibutylene fraction, hydrogenated is not considered as a PBT substance.

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 sources:

European Commission (2000a) IUCLID Dataset, Hydrocarbons, C4, 1,3-butadiene-free, polymd., dibutylene fraction, hydrogenated, CAS 93685-78-0, 19.2.2000.

European Commission (2000b) IUCLID Dataset, 2,2,4-trimethylpentane, CAS 540-84-1, 18.2.2000.

Other sources:

BP Chemicals Ltd. (2003) Personal communication to the Rapporteur.

MITI (1992) Biodegradation and Bioaccumulation data of Existing Chemicals based on CSCL Japan, Compiled under the Supervision of Chemical Products Safety Division, Basic Industries Bureau MITI, ed. by CITI, 1992. Published by Japan Chemical Industry Ecology-Toxicology & Information Center.