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., triisobutylene fraction, hydrogenated

EC number: 297-629-8

CAS number: 93685-81-5

Molecular formula: Not applicable

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 and T criteria as a borderline case. The screening P/vP criteria are fulfilled. The assessment was partly based on the main constituent 2,2,4,6,6-pentamethylheptane (CAS 13475-82-6).

.

JUSTIFICATION

1 IDENTIFICATION OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

Name:	Hydrocarbons, C4, 1,3-butadiene-free, polymd., triisobutylene fraction, hydrogenated
EC Number:	297-629-8
CAS Number:	93685-81-5
IUPAC Name:	
Molecular Formula:	Not applicable
Structural Formula:	Not applicable
Molecular Weight:	Not applicable
Synonyms:	2,2,4,6,6-pentamethylheptan

1.1 PURITY/IMPURITIES/ADDITIVES

According to industry, hydrocarbons, C4, 1,3-butadiene-free, polymd., triisobutylene fraction, hydrogenated consists of following constituents:

2,2,4,6,6-pentamethylpentane (CAS No. 13475-82-6): 85%

2,4,4,6,6-pentamethylheptane 5%

2,3,4,6,6-pentamethyheptane 3%

Other C12 hydrocarbons 7%

1.2 PHYSICO-CHEMICAL PROPERTIES

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

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		
VII, 7.3	Boiling point	176-192ºC at 1013 hPa	EC Erdölchemie (1994) (data not evaluated)
VII, 7.5	Vapour pressure	1 hPa (at 20ºC)	EC Erdölchemie (1994) (data not evaluated)
VII, 7.7	Water solubility	< 0.1 g l^{-1} (at 20ºC)	EC Erdölchemie (1994) (data not evaluated)
		0.151 mg l^{-1} (at 25ºC)	For 2,2,4,6,6-pentamethylheptane; WSKOW v1.41 using logKow of 5.94
		0.053 mg l^{-1}	SafePharm Laboratories (2004a); saturated *D. Magna* 21-d repro. test water
VII, 7.8	Partition coefficient n-octanol/water (log value)	6.4	For 2,2,4,6,6-pentamethylheptane with CLOGP; EC Erdölchemie (1994)
		5.94	For 2,2,4,6,6-pentamethylheptane; KOWWIN v1.67
	Dissociation constant	-	

2 MANUFACTURE AND USES

One company has provided information on the substance under Regulation 93/793/EEC.

3 CLASSIFICATION AND LABELLING

The 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

Indirect photochemical degradation of the main component 2,2,4,6,6-pentamethylheptane (CAS 13475-82-6) in the atmosphere is considered to be slow based on the estimated half-life of 2.3 days for the reaction with OH-radicals using AOP v1.91 (24-hour day^{-1}; $5*10^5$ OH^- cm^{-3}).

4.1.2 Biotic degradation

Bayer AG (1986) reports in the IUCLID (European Commission, 2000) a BOD_5/COD-ratio of < 0.2. No further details were provided on the result and it is noted that the report was not available to the Rapporteur for evaluation.

A ready biodegradability test according to OECD 301 D using triisobutylene (= pentamethylheptene; CAS 7756-94-7) as test substance and a test concentration of 1.5 mg l^{-1} resulted a degradation of 3% (as BOD) in 28 days (MITI, 1992). It is noted, that this substance is expected to be equally or faster biodegradable than its fully hydrogenated isomer 2,2,4,6,6-pentamethylheptane due to the unsaturated C-bond.

Exxon (1998) has reported on an OECD 301F –test using ISOPAR H (CAS 90622-57-4; PBT summary No. 24) as a test substance. This substance contains as main constituents C11 and C12-alkanes with approximately 5 methyl branches at most (average branching 3.25; see PBT summary No. 24). Using a non-acclimated inoculum, 6% had been degraded in 28 days, whereas with acclimated inoculum 16% at day 28 and 48% at day 90 had been degraded. It is noted, that the test report was not available to the Rapporteur for evaluation. The main difference of ISOPAR H and hydrocarbons, C4, 1,3-butadiene-free, polymd., triisobutylene fraction, hydrogenated is the degree of branching of the constituents. The degree of branching has impact mainly on the persistence of the substance (the more branches the less biodegradable). Hence, results from a similar test with hydrocarbons, C4, 1,3-butadiene-free, polymd., triisobutylene fraction, hydrogenated would be expected to show slower biodegradation than the results for ISOPAR H.

BIOWIN v4.02 provides for the main component 2,2,4,6,6-pentamethylheptane following biodegradation predictions:

BIOWIN 1: Does not biodegrade fast (0.299)
BIOWIN 2: Does not biodegrade fast (0.054)
BIOWIN 3: Weeks-months (2.399)
BIOWIN 4: Days-weeks (3.295)
BIOWNI 5: Does not biodegrade fast (0.392)
BIOWIN 6: Does not biodegrade fast (0.332).
Ready biodegradability prediction: not readily biodegradable

4.1.3 Other information [1]

No data available.

4.1.4 Summary and discussion of persistence

Based on the BOD_5/COD-ratio of the substance, the BIOWIN -predictions of the main constituent 2,2,4,6,6-pentamethylheptane and considering also the results of the ready biodegradation tests with triisobutylene and another branched alkane mixture ISOPAR H (which both are expected to degrade faster than hydrocarbons, C4, 1,3-butadiene-free, polymd., triisobutylene fraction, hydrogenated), the substance is concluded to be not readily biodegradable.

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

4.2 ENVIRONMENTAL DISTRIBUTION

Data not reviewed for this report.

4.2.1 Adsorption

4.2.2 Volatilisation

4.2.3 Long-range environmental transport

4.3 BIOACCUMULATION (B)

4.3.1 Screening data[2]

Estimated logKow –values of 6.4 and 5.94 are available for the main constituent 2,2,4,6,6-pentamethylheptane (see Table 1). A BCF of 7 464 was obtained with BCFWIN v2.17 using the logKow of 5.94. A BCF of 16 900 results using the logKow of 6.4.

4.3.2 Measured bioaccumulation data[3]

Tolls and van Dijk (2002) used the main constituent 2,2,4,6,6-pentamethylheptane as test substance in a flow-through bioconcentration test system designed to minimise the impact of the very high volatility and the high adsorption potential and to attain a stabile dissolved test concentration as close to the water solubility limit as possible. The fish (*Pimephales promelas)* were exposed over 12 days to the substance, concentration in fish was measured at days 2, 4, 8, 10, 11 and 12 and concentration in water daily. A rapid initial decrease of the exposure concentration from 17.7 to 3.5 µg l^{-1} was followed by a steady increase up to 9 µg l^{-1} at the end of the exposure. BCFs were determined for each fish sampling occasion as the ratio of concentration in whole fish to water. The concentration in fish seemed to reach a steady state within four days. A steady-state BCF of 880 ± 438 l kg^{-1} was determined as the mean BCF of the data of days 4 to 12. The authors considered, that the relatively low observed BCF compared to the predicted accumulation potential based on logKow would be caused by the capability of fish to metabolise this kind of hydrocarbons.

It is noted, that only one exposure aquarium was used (probably due to the complexity of the system), the number of fish sampled per sampling occasion was not indicated and the concentration variation between individual fish was very large but attributed by the authors to biological variation between the fish, not to the analytical procedure. Considering the difficulty to test this kind of substances, the good level of documentation, a relatively good stability of the test concentration compared to ecotoxicity tests described in section 6 and the fact that steady state was very obviously reached, the result is deemed reliable enough to be taken into account in this assessment.

Parkerton et al. (2001) have reported on a BCF of 3141 obtained with rainbow trout in a dietary accumulation test with pentamethylheptane (CAS 30586-18-6). No further details of the specific

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

[3] For example, fish bioconcentration factor

test are available. However, it is noted, that direct BCFs obtained from dietary tests may generally provide too conservative impression on the bioaccumulation potential.

4.3.3 Other supporting information[4]

No data available.

4.3.4 Summary and discussion of bioaccumulation

The main constituent 2,2,4,6,6-pentamethylheptane has based on a reliable flow through test a BCF of 880 ± 438 l kg^{-1} for fish. Additionally, a BCF of 3,141 is available from a dietary accumulation test with fish. These results are lower than the predicted values on the basis of logKow (7,464 and 16,900). The difference between the experimental and predicted values is probably caused by the ability of fish to metabolise this type of hydrocarbons. However, it is noted, that there is no information available on the bioaccumulation potential of the substance in aquatic organisms other than fish and analogous to PAHs (see e.g., European Commission, 2007), other animals may not have the capability to metabolise branched hydrocarbons as effectively. The other constituents of the substance are not expected to exhibit higher bioaccumulation potential. It can be concluded that the substance has a moderate to high bioaccumulation potential (in fish).

5 HUMAN HEALTH HAZARD ASSESSMENT

Data not reviewed for this report.

6 ENVIRONMENTAL HAZARD ASSESSMENT

6.1 AQUATIC COMPARTMENT (INCLUDING SEDIMENT)

ECOSAR v0.99h predicts the following acute values for 2,2,4,6,6-pentamethylheptane:

Fish: LC_{50} (96-hour) = 0.009 mg l^{-1}

Daphnid: LC_{50} (48-hour) = 0.013 mg l^{-1}

Green algae: EC_{50} (96-hour) = 0.011 mg l^{-1}

6.1.1 Toxicity test results

6.1.1.1 Fish

Acute toxicity

Hydrocarbons, C4, 1,3-butadiene-free, polymd., triisobutylene fraction, hydrogenated is a highly volatile substance with a very low water solubility. The IUCLID (European Commission, 2000)

[4]For example, measured concentrations in biota

contains two acute ecotoxicity test results with fish from static tests without test substance monitoring (Bayer AG, 1978 and 1972). The acute toxicity values reported are far beyond the water solubility of the substance. The test reports were not available to the Rapporteur for evaluation, but it is considered that the results as presented in the IUCLID are not reliable to make conclusions.

Long-term toxicity

6.1.1.2 Aquatic invertebrates

Acute toxicity

Long-term toxicity

SafePharm Laboratories (2004a) conducted a 21-day reproduction toxicity test for *Daphnia magna* following the OECD 211, under GLP and using as a test substance according to the report 2,2,4,6,6-pentamethylheptane (CAS 13475-82-6). The authors reported on an alternative identity of the test item as hydrocarbons, C4, 1,3-butadiene-free, polymd., triisobutylene fraction, hydrogenated (CAS 93685-81-5), with a purity of 85% and containing approximately 8% other pentamethylheptanes, 7% other C12-hydrocarbons and 0.2% C8 –hydrocarbons. Hence it is noted, that the identity of the test substance corresponds well with the composition of hydrocarbons, C4, 1,3-butadiene-free, polymd., triisobutylene fraction, hydrogenated as indicated in Section 1.1.

Semi-static system with a test medium renewal every 24 hours, temperature of approximately 21ºC and nominal test concentrations of 0.0025, 0.0050, 0.010, 0.020 and 0.040 mg l^{-1} were employed following preliminary solubility trials and a range finding test. The highest test concentration corresponded with the saturated dissolved concentration in the medium. Test concentrations were observed to decrease significantly after the renewal of the medium and the results are therefore based on measured concentrations. The concentration in the lowest exposure concentration decreased during each 24-hours to < LOQ (0.00132 mg l^{-1}), whereas in other exposure levels the concentration mainly remained > LOQ and in the highest three exposure levels approximately 20-40% of the nominal concentration was generally found before the renewal of the medium (after the renewal > 80% of nominal found).

A NOEC (21-day) of 0.013 mg l^{-1} was determined for parent immobilisation and reproduction based on mean measured concentrations. An EC_{50} (21-day) of 0.20 mg l^{-1} for parent immobilisation was observed based on mean measured concentrations.

The study is considered well documented and the results reliable despite the problems to sustain stabile test concentrations.

6.1.1.3 Algae and aquatic plants

SafePharm Laboratories (2004b) carried out a static algal growth inhibition test according to OECD 201 under GLP with *Scenedesmus supspicatus*. For the test substance identity, see the above described Daphnia –test of SafePharm Laboratories (2004a). Following preliminary solubility trials, a range finding test with nominal concentrations of 0.0050, 0.050 and 0.50 mg l^{-1} were employed, where 0.50 mg l^{-1} was a saturated dissolved concentration in the test medium. A test concentration of the definite (limit) test was chosen as 0.40 mg l^{-1}. Duration of exposure was 168 hours and took place in 24 ± 1ºC. Samples were taken at 0, 24, 48, 72, 96, 120, 144 and 168 hours. Several controls and exposure replicates were run to take into account the volatility of the substance. pH of 8.4 measured at the start of the test increased to pH 9.7 at 72 hours and to 11.8-11.9 by the end of the

test. The cell growth between 0 and 72 hours in the controls complied with the test standard. Analysis of the unopened exposure controls showed that the test concentration was at the start 90 to 97% of the nominal 0.40 mg l^{-1} but had declined at the end of exposure to < LOQ (0.0022 mg l^{-1}).

No effects were observed at any time point (or in the range finding test at any test concentration). A "worst case" NOEC (0-168 hours) was determined at > 0.0064 mg l^{-1} based on geometric mean measured concentrations (at 0, 72 and 168 hours; results < LOQ treated as 0.5 × LOQ). Due to the instability of the substance the "worst case" –result should be considered as the final result.

The study is considered well documented and valid when considering the measured data as the basis for the determination of the NOEC (nominal concentrations should not be accounted for from this study).

6.1.2 Sediment organisms

No data available.

6.1.3 Other aquatic organisms

No data available.

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., triisobutylene fraction, hydrogenated fulfils the P/vP screening criteria. A BOD5/COD ratio of < 0.2 is available for the substance. Additionally, QSAR predictions of its main constituent 2,2,4,6,6-pentamethylheptane (CAS 13475-82-6) and results from an OECD 301D-test with a similar substance triisobutylene (CAS 7756-94-7) and from an OECD 301F –test with another branched alkane mixture ISOPAR H (CAS 90622-57-4, PBT summary No. 24), which both are expected to biodegrade faster than Hydrocarbons, C4, 1,3-butadiene-free, polymd., triisobutylene fraction, hydrogenated, indicate, that the substance is not readily biodegradable. Based on the results it seems that this kind of hydrocarbons are persistent in the environment and it is unlikely, that further testing would change the conclusion.

Bioaccumulation: The substance does not meet the B criterion as a borderline case. An experimental BCF of 880±438 l kg^{-1} was obtained for fish in a flow-through test for the main constituent 2,2,4,6,6-pentamethylheptane. It is generally known, that the fish are able to metabolise effectively this kind of hydrocarbon substances. However, it is noted, that no bioaccumulation data

with other animals are available and they may not be able to metabolise these substances as effectively as fish (analogous to PAHs).

Toxicity: The substance does not meet the T criterion as a borderline case. Experimental reliable long-term data are available for the main constituent 2,2,4,6,6-pentamethylheptane for *Daphnia magna* with a NOEC (21 days) of 0.013 mg l^{-1} from a semi-static OECD 211 -test. Additionally, no effects were observed in a static algal inhibition test according to OECD 201 at a nominal (and initial measured) concentration of 0.40 mg l^{-1} ("worst case" NOEC (0-168 hours) > 0.0064 mg l^{-1} based on measured concentrations). According to ECOSAR v0.99h, fish ecotoxicity is not expected to differ significantly from the ecotoxicity to invertebrates and algae. Additionally, the substance is due to its structure not expected to elicit effects beyond the baseline toxicity.

Summary: Hydrocarbons, C4, 1,3-butadiene-free, polymd., triisobutylene fraction, hydrogenated does not meet the B and T criteria as a borderline case. The substance meets the screening P/vP criteria. Part of the assessment was based on the data of the main constituent 2,2,4,6,6-pentamethylheptane (CAS 13475-82-6). It is concluded that hydrocarbons, C4, 1,3-butadiene-free, polymd., triisobutylene fraction, hydrogenated is not considered as a PBT substance (as a borderline case).

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 (2007) European Union Risk Assessment Report, Draft of January 2007, Coal tar pitch, high temperature, CAS No: 65996-93-2, EINECS No: 266-028-2.

European Commission (2000) IUCLID Dataset, Hydrocarbons, C4, 1,3-butadiene-free, polymd., triisobutylene fraction, hydrogenated, CAS 93685-81-5, 19.2.2000.

Exxon Biomedical Sciences Inc. (1998) Study 158894A(2), Ready Biodegradability: OECD 301F, Manometric Respirometry Test. Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA. (as cited in: CEFIC comments 12 February 2003).

Exxon Biomedical Sciences Inc. (1997) Study 156194A, Ready Biodegradability, Manometric Respirometry Test. Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA, (as cited in: CEFIC comments 12 February 2003).

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.

Parkerton T, Letkinski D, Febbo E, Davi R, Dzamba C, Connelly M, Christensen K And Peterson D (2001) A practical testing approach for assessing bioaccumulation potential of poorly water soluble organic chemicals. Presentation at SETAC Europe, Madrid.

SafePharm Laboratories (2004a) 2,2,4,6,6-pentamethylheptane: *Daphnia magna* reproduction test, SPL Project Number: 599/090. Study Sponsor: PB Chemicals Ltd, Middlesex, LN.

SafePharm Laboratories (2004b) 2,2,4,6,6-pentamethylheptane: Algal inhibition test, SPL Project Number: 599/089. Study Sponsor: PB Chemicals Ltd, Middlesex, LN.

Tolls J and van Dijk J (2002) Bioconcentration of n-dodecane and its highly branched isomer 2,2,4,6,6-pentamethylheptane in fathead minnows. Chemosphere, 47(10), 1049-1057.