TC NES SUBGROUP ON IDENTIFICATION OF PBT AND VPVB SUBSTANCES

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

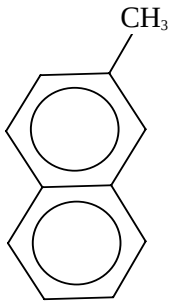
Substance name: 2-methylnaphthalene

EC number: 202-078-3

CAS number: 91-57-6

Molecular formula: C11H10

Structural formula:



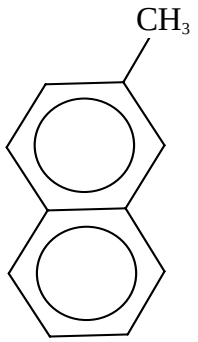
Summary of the evaluation:

The substance is not considered to be a PBT substance. It does not meet the B criterion. It clearly meets the P (and vP) criteria. The assessment of ecotoxicity was not completed.

JUSTIFICATION

1 IDENTIFICATION OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

Name: 2-methylnaphthalene
EC Number: 202-078-3
CAS Number: 91-57-6
IUPAC Name:
Molecular Formula: C11H10
Structural Formula:



Molecular Weight: 142.2
Synonyms: Naphthalene, 2-methyl-

1.1 PURITY/IMPURITIES/ADDITIVES

No data available for CAS number 91-57-6.

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		
V, 5.2	Melting / freezing point		
V, 5.3	Boiling point		
V, 5.5	Vapour pressure		
V, 5.7	Water solubility	41.4 mg l^{-1} at 25ºC 24.6 mg l^{-1} at 25ºC	Calculated (WSKOW v1.41) WSKOW v1.41 exper. database (Yalkowsky and Dannenfelser, 1992)(data not evaluated)
V, 5.8	Partition coefficient n-octanol/water (log value)	3.72 3.86	Calculated (KOWWIN v1.67) KOWWIN exper. database (Hansch et al., 1995)(data not evaluated)
VII, 5.19	Dissociation constant		

2 MANUFACTURE AND USES

One producer is operating in the EU-15 according to data provided under Regulation 93/793/EEC. 2-methylnaphthalene is a LPV substance. It is also contained in the HPV chemical methylnaphtalene (CAS 1321-94-4) (Ruetgerswerke AG, 1995).

3 CLASSIFICATION AND LABELLING

2-methylnaphthalene is not classified in the Annex I of the Directive 67/548/EEC.

4 ENVIRONMENTAL FATE PROPERTIES

4.1 DEGRADATION (P)

4.1.1 Abiotic degradation

Methylnaphthalenes undergo photodegradation in water. Experimental half-lives obtained in radiation conditions optimal for degradation (40ºN, summer, noon) are 3.7 hours for 2-methylnaphthalene and 3.6 hours for 1-methylnaphthalene (Zepp and Schlotzhauer, 1979). It is nevertheless considered, that photodegradation in water is not relevant for the assessment of persistency as photodegradation can only occur in the first few centimetres depth of the water column and because 2-methylnaphthalene is mainly distributed to sediment (and soil).

Indirect photochemical degradation in the atmosphere is considered to be fast based on the estimated half-life of 0.3 hours for the reaction with OH-radicals using AOP v1.91 (24-hour day^{-1}; $5 \cdot 10^5$ [OH] cm^{-3}).

4.1.2 Biotic degradation

2-methylnaphthalene was not readily biodegradable in a MITI I test (Yoshida et al., 1983). An inherent biodegradability test (MITI II) showed degradation of 71% after 21 days (Yoshida et al., 1983), but volatilisation may have influenced the results, which are thus not considered plausible.

Heitkamp and Cerniglia (1987) measured biodegradation of ^{14}C-labelled 2-methylnaphthalene in microcosms by monitoring the evolution of CO_2. The substance was added to sediment-water mixtures (1:10) for which the sediments had been sampled from a contaminated estuary site, a contaminated lake site and a relatively pristine lake. Half-lives of 98 days, 112 days and 140 days were determined, respectively.

Pruell and Quinn (1985) measured degradation of 2-methylnaphthalene and other PAHs in mesocosms of MERL type by monitoring the test substance concentrations. Three sediments sampled along a contaminant gradient in an estuary (Rhode Island, U.S.) were employed for 394 days. Degradation half-life for the most contaminated sediment was 353 days, whereas the concentration did not change during the experiment in the two less contaminated sediments. For 1-methylnaphthalene a half-life of 321 days was determined.

Lee and Ryan (1981) studied biodegradation of ^{14}C-labelled 2-methylnaphthalene in water measuring the evolution of CO_2. For water collected from an estuarine in Rhode Island (U.S.), and contained before the incubation together with sediment in mesocosms, half-lives of 530 days (at 7ºC, test concentration 25 µg l^{-1}), 390 days (at 7ºC, test concentration 10 µg l^{-1}) and 53 days (at

23ºC, test concentration 25 µg l^{-1}) were extrapolated. For water samples from mesocosms with oil treatment much lower half-lives were obtained. Water samples from two heavily contaminated estuarines were also tested (test concentration 25 µg l^{-1}) and half-lives between 3 days (at 28ºC) and 57 days (at 8ºC) were determined.

4.1.3 Other information [1]

Methylnaphthalenes are ubiquitous in Arctic and Antarctic sediments . This presence is connected to oil releases in these regions (AMAP, 1998).

4.1.4 Summary and discussion of persistence

The available studies indicate that 2-methylnaphthalene is degraded by adapted micro-organisms, but that the degradation in conditions more relevant for the environment is very slow according to half-lives determined (DT_{50} = 140 days for lake sediment, DT_{50} > 352 days for estuarine sediment, DT_{50} 53-530 days for estuarine water). 2-methylnaphthalene degrades fast in atmosphere (DT_{50} is 0.3 days).

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

2-methylnaphthalene does not have potential for long-range atmospheric transport in vapour phase due to its short half-life in the atmosphere.

4.3 BIOACCUMULATION (B)

4.3.1 Screening data[2]

On the basis of octanol-water partitioning (logKow 3.7 and 3.86 available), moderate bioaccumulation potential is expected for 2-methylnaphthalene. A BCF of 141 was estimated by BCFWIN v2.15 using logKow of 3.86.

4.3.2 Measured bioaccumulation data[3]

Following experimental data on bioaccumulation have been available to the Rapporteur for evaluation (see **Table 4.1**).

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

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

3 For example, fish bioconcentration factor

Table 4.1 Experimental bioaccumulation data.

Species	BCF	Comment	Reference
Fish			
Oncorhynchus kisutch	30 – 190 (dry weight)	Muscle tissue; depuration half-life 2 days	Roubal et al. (1978)
Platichtys stellatus	110 – 2,800 (dry weight)	Muscle tissue; Methylnaphthalene introduced into the test vessels along other PAHs in Prudhoe crude oil	
	1,000 – 2,000 (dry weight; during exposure) 300 (dry weight; after depuration)	Liver tissue; Methylnaphthalene introduced into the test vessels along other PAHs in Prudhoe crude oil	
	400 – 770 (dry weight)	Gills; Methylnaphthalene introduced into the test vessels along other PAHs in Prudhoe crude oil	
Salmo gairdneri	100 – 300 (steady state; wet weight)	Results of muscle, blood and liver (measured separately); duration 28 days	Melancon and Lech (1978)
	23,500	Bile	
Other			
Crassostera virginica	7,000 – 12,000 (BAF)	Depuration half-life 2 days; mesocosm study; methylnaphthalene introduced into the test vessels along other PAHs in Prudhoe crude oil; isomers not specified	Lee et al. (1978)

The highest BCFs for fish are from the study of Roubal et al. (1978) where the results were expressed in relation to dry weight. It is not possible on the basis of the study report to normalise the results to wet weight but it can be expected that the BCFs on wet weight basis would be significantly lower.

4.3.3 Other supporting information[4]

Pereira et al. (1996) measured prevailing concentrations of 2-methylnaphthalene in water and benthic filter feeding Asian clam *Corbicula fluminea* in a Californian river. The clams were depurated 48 hours before analysis. A field BAF (bioaccumulation factor) of 143 can be estimated from the study as a relation of measured concentrations in clam and water. The BAF may be slightly underestimated since water samples were only centrifuged (not filtered) before measuring the concentration.

4.3.4 Summary and discussion of bioaccumulation

The experimental data on BCFs for several fish tissues evaluated by the Rapporteur, the available logKow-values and the estimated BCF indicate moderate bioaccumulation potential. The bioaccumulation observed in oysters is very high but an estimated field BAF for Asian clam is also in the line with the fish data.

5 HUMAN HEALTH HAZARD ASSESSMENT

Data not reviewed for this report.

[4]For example, measured concentrations in biota

6 ENVIRONMENTAL HAZARD ASSESSMENT

6.1 AQUATIC COMPARTMENT (INCLUDING SEDIMENT)

6.1.1 Toxicity test results

In general, L(E)C_{50} of approximately 1-10 mg l^{-1} have been measured for fish, invertebrates and algae but also lower results are available. The assessment of ecotoxicity was not completed.

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

6.3 ATMOSPHERIC COMPARTMENT

7 PBT AND VPVB

7.1 PBT, VPVB ASSESSMENT

Persistence: Biodegradation studies conducted in conditions relevant for the environment have determined a half-life of 140 days for freshwater sediment, half-life > 352 days for estuarine sediment and half-lives up to 530 days for estuarine water. The studies indicate that 2-methylnaphthalene degrades if pre-adapted micro-organisms are employed but that it persists very long in tests with non-adapted material. It is concluded that 2-methylnaphthalene fulfils the P (and vP) criteria.

Bioaccumulation: Several experimental BCFs for fish are available which all are clearly below 2000. In addition, the available logKow –values, the BCF estimated using a QSAR-model and a field BAF for clams also point to low bioaccumulation potential, although the very high

bioaccumulation observed in oysters give reason to some concern. On the basis of the available data, 2-methylnaphthalene is concluded not to meet the B criterion.

Toxicity: The assessment of ecotoxicity was not completed.

Summary: 2-methylnaphthalene fulfils the P (and vP) criteria on the basis of several biodegradation conducted studies in conditions relevant to the environment. The substance does not meet the B criterion according to the available data. The assessment of ecotoxicity was not completed.

INFORMATION ON USE AND EXPOSURE

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

OTHER INFORMATION

The information and references used in this report are included in the following reports:

GDCh (1990) BUA Stoffbericht Nr. 47: Methylnaphthaline, CAS-Nr.: 90-12-0 (1), 91-57-6 (2), 581-42-0 (2,6). Edited by GDCh-Advisory Committee on Existing Chemicals of Environmental Relevance (BUA). ISBN 3-527-28224-6.

Ruetgerswerke AG (1995) Confidential IUCLID data set, Methylnaphthalene (CAS 1321-94-4), 08.03.1995.

Other sources:

AMAP (1998) AMAP Assessment Report, Arctic Pollution Issues, 682-984.

Pereira WE, Domagalski JL, Hostettler FD, Brown LR and Rapp JB (1996) Occurrence and accumulation of pesticides and organic contaminants in river sediment, water and clam tissues from the San Joaquim River and tributaries, California. Environmental Toxicology and Chemistry, 15(2), 172-180.