TC NES SUBGROUP ON IDENTIFICATION OF PBT AND VPVB SUBSTANCES

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

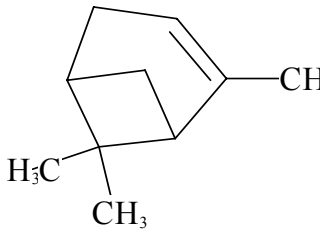
Substance name: Terpenes and Terpenoids, turpentine-oil, alpha-pinene fraction

EC number: 266-031-9

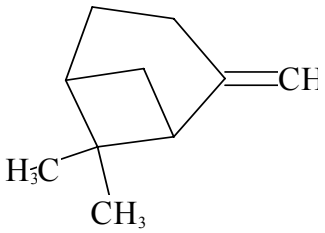
CAS number: 65996-96-5

Molecular formula: C10H16

Structural formula:



α-pinene (CAS 80-56-8 and 7785-70-8)



β-pinene (CAS 127-91-3)

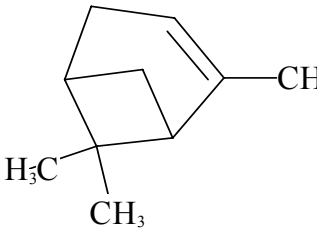
Summary of the evaluation:

Terpenes and terpenoids, turpentine-oil, alpha-pinene fraction is not considered as a PBT substance based on mainly screening data. Its constituents α-pinene and β-pinene do not meet the P/vP criteria according to screening data. B criterion is neither fulfilled based on screening data but the conclusion is supported by an experimental BCF for a structurally similar substance (camphene). β-pinene is concluded to not fulfil the T criterion. α-pinene does not meet the T criterion based on read-across from β-pinene.

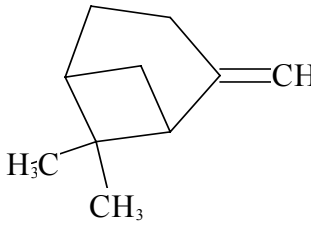
JUSTIFICATION

1 IDENTIFICATION OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

Name: Terpenes and Terpenoids, turpentine-oil, alpha-pinene fraction
EC Number: 266-031-9
CAS Number: 65996-96-5
IUPAC Name:
Molecular Formula: C10H16
Structural Formula:



α-pinene (CAS 80-56-8 and 7785-70-8)



β-pinene (CAS 127-91-3)

Molecular Weight: 136.24
Synonyms: Alpha-pinene ; Oulu 402, Oulu 402SF

1.1 Purity/impurities/additives

According to the only European producer, alpha-pinene fraction consists mainly of α-pinene (CAS 80-56-8 and 7785-70-8) and has β-pinene (CAS 127-91-3) as a minor constituent. It is not common that alpha-pinene fraction would contain other constituents or relevant impurities. Finnish Chemicals Industry (1990) reports that α-pinene would make 96% w/w of the substance. In the Merck Index (1996) the substance contains 92-97% α-pinene and 1-7% β-pinene.

1.2 Physico-chemical properties

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

REACH ref Annex, §	Property	Value	Comments
V, 5.1	Physical state at 20 C and 101.3 Kpa	liquid	
V, 5.2	Melting / freezing point	-	
V, 5.3	Boiling point	162-174°C at 1013 hPa	Forchem Oy (data not evaluated)
V, 5.5	Vapour pressure	2 hPa at 20°C	Forchem Oy; for δ-carene (data not evaluated)
V, 5.7	Water solubility	"insoluble"	Forchem Oy (data not evaluated)
V, 5.8	Partition coefficient n-octanol/water (log value)	4.5-5.5 (at 35°C) at pH 2	OECD 117; Forchem Oy (data not evaluated)
VII, 5.19	Dissociation constant	-	

Water solubility and logKow of the two constituents are presented in **Table 4.2** in Section 4.3.

2 MANUFACTURE AND USES

One company has notified the substance under Regulation 93/793/EEC. The raw material of the substance is turpentine ("turpentine oil", "raw turpentine"), which is captured from process vapours of steaming and cooking phases in pulp mills. According to Gullichen and Fogelholm (1999), the purity of turpentine varies depending on at which phase of the pulping process it is obtained. Steaming phase produces the purest fraction. Variation of the contents can be also expected to be caused by the quality variation in the raw material (softwood).

Turpentine is further distilled to gain monoterpene fractions like alpha-pinene fraction, beta-pinene fraction, delta-carene fraction and gum turpentine. Distillate residues contain higher boiling terpenes, terpenalcohols and sesquiterpenes (Gullichen and Fogelholm, 1999).

3 CLASSIFICATION AND LABELLING

The substance is not classified under Directive 67/548/EEC.

4 ENVIRONMENTAL FATE PROPERTIES

4.1 Degradation (P)

4.1.1 Abiotic degradation

Monoterpenes like α-pinene and β-pinene are not expected to be susceptible to hydrolysis in surface water. In the atmosphere, these compounds react with free radicals and ozone formed in the

atmosphere from ions, such as nitrate, chloride, and ammonium, in the presence of sunlight (Corchnoy and Atkinson 1990). Calculated T½ in the air for α-pinene is less than 3 hours (AOPWIN v 1.92). This abiotic degradation evaluation relies on secondary sources and no measured abiotic degradation study reports were evaluated or located under this assessment

4.1.2 Biotic degradation

The available data on biodegradation of the two constituents and of other monoterpenes are listed in **Table 4.1**.

Table 4.1 Persistency of the constituents in alpha-pinene fraction and of other monoterpenes

	BIOWIN 2 v4.02	BIOWIN 3 v4.02	BIOWIN 6 v4.02	Experimental data	Screening (v)P criteria fulfilled? (see also Section 4.1.4)
α-pinene (CAS 80-56-8)	0.34	2.69	0.33	Readily biodegradable. 62% mineralisation in 28 days, 70% in 42 days; OECD 301B, closed bottles used (Astra Zeneca, 2004a)	No
β-pinene (CAS 127-91-3)	0.34	2.69	0.39	No data on pure substance. In a test with gum turpentine fraction (50.8% α-pinene, 36.8% β-pinene), 52% mineralisation in 28 days was observed; OECD 301B-test, closed bottles used (Astra Zeneca, 2001).	No (at limit)
δ-carene (CAS 13466-78-9)	0.34	2.69	0.33	Not readily biodegradable. 53% mineralisation in 28 days, 74% in 42 days; OECD 301B, closed bottles used (Astra Zeneca, 2004b). Degradation curve did not reach plateau at day 42. δ-carene can be considered as biodegradable.	No (at limit)
camphene (CAS 79-92-5)	0.34	2.69	0.39	Not readily biodegradable. 1-4% in 28 days in an OECD 301C -test (MITI 1992). Other test –results cited in European Commission (2000c) support the result (data not evaluated)	Yes
limonene/dipentene (CAS 5989-27-5)	0.75	2.90	0.33	Readily biodegradable. > 70% degradation in 28 days in an OECD 301C –test (MITI 1992).	No

4.1.3 Other information [1]

No data available.

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

4.1.4 Summary and discussion of persistence

The available standard ready biodegradability test of Astra Zeneca (2004a) with pure α-pinene shows that the substance is readily biodegradable. For β-pinene no test data are available on pure substance. When comparing the results of the ready biodegradability test using gum turpentine (Astra Zeneca, 2001) with the results obtained for pure α-pinene, it can be concluded that β-pinene did not slow down the biodegradation significantly in the test with gum turpentine. It must also be noted, that the test measured ultimate mineralisation. Hence, it is concluded that also β-pinene is considered biodegradable. Results from standard ready biodegradability tests with two other monoterpenes δ-carene and limonene support this conclusion.

The applicability of BIOWIN for monoterpenes is questionable, because the program does not calculate any fragment corrections for specific substructure entities and uses instead a molecular weight parameter. The quaternary carbons are identified as "carbon with 4 single bonds and no hydrogens" without distinguishing the cyclic structure they are connected with.

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

The available screening data on water solubility, logKow and bioaccumulation for α-pinene, β-pinene and other monoterpenes are presented in **Table 4.2**.

Table 4.2 Water solubility, logKow and BCF of the constituents and other monoterpenes

	Water solubility (mg l^{-1} at 25 ºC)	LogKow	BCF	B/vB criterion fulfilled? (see also Section 4.3.3)
α-pinene	4.07 (WSKOW v1.41) 2.49 (Li and Perdue, 1995 in WSKOW exper. database)	4.27 (KOWWIN v1.67) 4.83 (Li and Perdue, 1995 in KOWWIN exper. database)	1,045 (BCFWIN v2.15 using logKow of 4.83)	No (screening data)
β-pinene	7.06 (WSKOW v1.41)	4.35 (KOWWIN v1.67) 4.16 (Griffin et al., 1999, in KOWWIN exper. database)	446 (BCFWIN v2.15 using logKow of 4.35)	No (screening data)
δ-carene	4.58 (WSKOW v1.41)	4.61 (KOWWIN v1.67) 4.38 (Griffin et al., 1999, in KOWWIN exper. database)	708 (BCFWIN v2.15 using logKow of 4.61)	No (at the limit; screening data)
camphene	6.27 (WSKOW v1.41) 4.6 (Chem Inspect Test Inst in WSKOW exper. database) 4.2 (at 20ºC; Hoechst AG, 1991 in European Commission, 2000c; data not evaluated)	4.35 (KOWWIN v1.67) 4.22 (Griffin et al., 1999, in KOWWIN exper. database)	446 (BCFWIN v2.15 using logKow of 4.35) 606-1,290 (MITI, 1992; OECD 305 with *Cyprinus carpio*, test conc. 1.5 mg l^{-1})	No
limonene/dipentene	4.58 (WSKOW v1.41) 13.8 (Massaldi and King, 1979 in WSKOW exper. database)	4.83 (KOWWIN v1.67) 4.57 (Li and Perdue, 1995 in KOWWIN exper. database) 4.38 (Griffin et al., 1999, in KOWWIN exper. database)	1,045 (BCFWIN v2.15 using logKow of 4.83)	No (screening data)

4.3.2 Measured bioaccumulation data

No experimentally derived bioaccumulation data are available for α-pinene and β-pinene. An experimental BCF has been derived for camphene (see **Table 4.2**).

4.3.3 Other supporting information[2]

No data available.

4.3.4 Summary and discussion of bioaccumulation

Experimental data on bioaccumulation are for the group of monoterpenes available only for camphene. All monoterpenes are expected to have a moderate to high bioaccumulation potential based on their BCFWIN –estimates and logKow-values. For β-pinene both the logKow–values and the BCFWIN –estimate indicate that it does not meet the B criterion. One of the two available logKow–values for α-pinene is slightly higher than the screening criterion of 4.5. However, it is considered that BCFWIN estimates for monoterpenes are in line with the BCFWIN-estimate and the measured BCF for camphene. Therefore BCFWIN estimates of monoterpenes are considered reliable enough to conclude that these substances are not likely to exceed the B criterion. Further bioaccumulation testing of monoterpenes is not needed in the frame of this assessment.

5 HUMAN HEALTH HAZARD ASSESSMENT

Data not reviewed for this report.

6 ENVIRONMENTAL HAZARD ASSESSMENT

Table 6.1 presents the available ecotoxicity data on the constituents and other monoterpenes. Long-term ecotoxicity test results are available for β-pinene. Due to the similarity of α-pinene and β-pinene it is considered that the outcome is applicable also to α-pinene.

[2]For example, measured concentrations in biota

Table 6.1 Ecotoxicity of α-pinene, β-pinene and other monoterpenes. The results have been cited in European Commission (2000a,b,c) and partly in confidential IUCLIDs

	Ecotoxicity
α-pinene	Only short-term data are available. With pure substance: 96-hour LC_{50} = 0.28 mg l^{-1} *Pimephales promelas* (Union Camp Corporation, 1992) 96-hour LC_{50} = 1 mg l^{-1} *Chaetogammarus marinus* (NOEC 0.18 mg l^{-1}) (Arizona Chemicals) 48-hour EC_{50} = 41 mg l^{-1} *Daphnia magna,* (Leblanc,1980) Several test results with gum turpentine mixture containing α-pinene are also available.
β-pinene	48-hour EC_{50} = 1.25 mg l^{-1} Daphnia 48-hour EC_{50} = 1.44 mg l^{-1} Green algae 60-day LOEC = 320 µg l^{-1} (growth, rainbow trout fry)
δ-carene	No data on pure substance available.
camphene	48-hour LC_{50} = 2 mg l^{-1} , fish (MITI, 1992) 48-hour LC_{50} <1.8 mg l^{-1} 72-hour LC_{50} < 2 mg l^{-1} 96-hour LC_{50} <0.19 mg l^{-1}
limonene/dipentene	-

6.1 Aquatic compartment (including sediment)

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

No data available.

6.1.3 Other aquatic organisms

Data not evaluated for this report.

6.2 Terrestrial compartment

No data available.

6.3 Atmospheric compartment

No data available.

7 PBT AND vPvB

7.1 PBT, vPvB assessment

Terpenes and Terpenoids, turpentine-oil, alpha-pinene fraction ("alpha-pinene fraction") contains two constituents (α-pinene and β-pinene). An overview and conclusion of the PBT-properties is presented in **Table 7.1**. The available data have been presented and discussed in **Sections 4.1**, **4.3** and **6**.

Table 7.1 Overview of the PBT-properties of α-pinene and β-pinene

	P/vP criteria fulfilled?	B/vB criteria fulfilled?	T criteria fulfilled?	Overall conclusion
α-pinene	No (screening data, measured)	No (screening data, estimated BCF but supported by experimental BCF of another monoterpene)	Long term data not available (acute data > 0.1 mg l^{-1}; not T based on read-across from β-pinene)	Not PBT (based on mainly screening data)
β-pinene	No (at limit; screening data, measured)	No (screening data, estimated BCF but supported by experimental BCF of another monoterpene)	No (long-term data available)	Not PBT (based on mainly screening data)

Summary: Terpenes and Terpenoids, turpentine-oil, alpha-pinene fraction does not meet the PBT criteria based on mainly screening data. Its constituents α-pinene and β-pinene do not meet the P/vP criteria according to screening data. B criterion is neither fulfilled based on screening data, but the conclusion is supported by an experimental BCF for a structurally similar substance (camphene). β-pinene is concluded to not fulfil the T criterion. α-pinene does not meet the T criterion based on read-across from β-pinene It is concluded that terpenes and terpenoids, turpentine-oil, alpha-pinene fraction 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 taken from the following sources:

Astra Zeneca (2004a) Alpha-pinene: Determination of Ready Biodegradability (CO_2 evolution). Report nr. BLS3163/B provided with Arizona Chemicals communication on 16.4.2004.

Astra Zeneca (2004b) Delta-3-carene: Determination of Ready Biodegradability (CO_2 evolution). Draft report nr. BLS3164/B. Arizona Chemicals communication on 16.4.2004.

Astra Zeneca (2001) Secondary source Report nr. BL7034/B/2001 provided with Arizona Chemicals written comment to Finnish CA (10 Feb 2003).

European Commission (2000a) IUCLID Dataset, Terpenes and Terpenoids, turpentine-oil, alpha-pinene fraction, CAS 65996-96-5, 19.2.2000.

European Commission (2000b) IUCLID Dataset, Terpenes and Terpenoids, turpentine-oil, 3-carene CAS 91770-80-8, 19.2.2000.

European Commission (2000c) IUCLID Dataset, Camphene CAS 79-92-5, 19.2.2000.

Finnish Chemicals Industry (1990) Publisher: Kemian keskusliitto & Chemas Oy Mikkeli 1990, ISBN 952-9597-02-9

Gullichen J and Fogelholm C-J (1999) Chemical Pulping, in scientific series of Papermaking Science and Technology, publication 6b, Helsinki 1999

Merck & Co. Inc. (1996) Merck Index, 12th edition, Ed. Susan Budavari Whitegouse Station, NJ.

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.