TC NES SUBGROUP ON IDENTIFICATION OF PBT AND VPVB SUBSTANCES

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

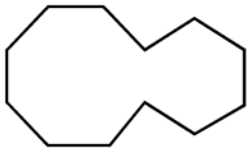
Substance name: Cyclododecane

EC number: 206-033-9

CAS number: 294-62-2

Molecular formula: C12H24

Structural formula:



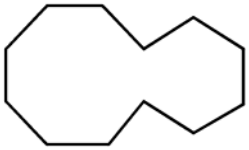
Summary of the evaluation:

Cyclododecane is considered to be a PBT and vPvB substance based on the screening criteria. The substance fulfils the vB criterion. The P/vP screening criterion and the T screening criterion are also met. No further testing is proposed at the present as the substance is mainly used as intermediate.

JUSTIFICATION

1 IDENTIFICATION OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

Name: Cyclododecane
EC Number: 206-033-9
CAS Number: 294-62-2
IUPAC Name:
Molecular Formula: C12H24
Structural Formula:



Molecular Weight: 168.33
Synonyms:

1.1 Purity/impurities/additives

No relevant impurities.

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 solid	
V, 5.2	Melting / freezing point	61ºC	Hüls AG (1979). Study not evaluated.
V, 5.3	Boiling point	244ºC at 1013 hPa	Meyer and Hotz (1975). Study not evaluated.
V, 5.5	Vapour pressure	0.07 hPa at 20ºC	Meyer and Hots (1976). Study not evaluated.
V, 5.7	Water solubility	< 1 mg l^{-1} 10 mg l^{-1} 0.11 mg l^{-1}	MITI (1992) Sicherheitsdatenblatt Huels AG. Study not evaluated. WSKOW v1.41
V, 5.8	Partition coefficient n-octanol/water (log value)	> 6.19 6.12 (calculated) 6.7 (calculated)	MITI (1992) KOWWIN v1.67 CLOGP3 by Huels AG Marl
VII, 5.19	Dissociation constant	-	

2 MANUFACTURE AND USES

Two producers operate in the EU at the present. Cyclododecane is used almost exclusively as intermediate. According to the producers, the intermediate use occur mainly in closed systems. Several sources report also the use as a fixative for conservation purposes (e.g. Hangleiter GmbH, 2006 and Kremer Pigments, 2006). The use volume for this purpose can be expected to be low.

3 CLASSIFICATION AND LABELLING

This 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

Reaction half-life with OH-radicals in the atmosphere was estimated at 22.7 hours by AopWin v1.91 ($5*10^5$ OH cm^{-3}; 24 h day^{-1}). No estimate for reaction with ozone was provided by the model.

4.1.2 Biotic degradation

According to MITI (1992), 0-12% of the substance was degraded after 14 days in a ready biodegradability test with a test substance concentration of 100 mg l^{-1} and a sludge concentration of 30 mg l^{-1}.

Following tests with non-adapted micro-organisms are cited in the available IUCLIDs (European Commission, 2000; Degussa AG, 2002). A closed bottle test according to the OECD 301 D guideline (Huels-Untersuchung, unveröffentlicht) resulted in 3% degradation in 28 days. In a BODIS test according to ISO 10708 (in preparation) degradation of 18% after 28 days was observed (Huels-Untersuchung, unveröffentlicht). In addition, no degradation was detected in 28 days in a modified Sturm test (C.5. of 84/448/EEC; Hüls AG 1997). These results were not evaluated by the Rapporteur as the reports were not available.

Azolay et al. (1983) observed that two of five bacterial strains isolated from Mediterranean sediment from a polluted site grew well using cyclododecane as the sole carbon source. In a test employing a mixed bacterial sediment population from the same polluted site 30% of cyclododecane in a hydrocabon mixture was degraded after 8 days of incubation at 30ºC. Degradation in sediment from unpolluted site was used as reference. In addition, Schumacher and Fakoussa (1999) concluded that *Rhodococcus ruber* CD4 was oxidising cyclododecane as the sole carbon source at 28ºC. Cyclododecane was shown to be oxidized to cyclododecanol and cyclododecanone, followed by ring fission. The resulting lactone gives rise to an omega-hydroxyalkanoic acid which is further degraded by common beta-oxidation.

4.1.3 Other information [1]

BIOWIN v4.02 gives an overall prediction that the substance is not readily biodegradable. However, some degradation is expected to occur according to the models.

4.1.4 Summary and discussion of persistence

Based on the available ready biodegradability test results, cyclododecane is considered not readily biodegradable. Very slow or no degradation at all was observed in the tests. Cyclododecane has been shown to be degraded by adapted inocula with mixed microbial population and by specific strains.

Based on the available information it is likely that the substance is very persistent in the environment. Further testing would be needed to determine the rate of degradation.

4.2 Environmental distribution

4.2.1 Adsorption

Adsorption was not assessed for this substance.

4.2.2 Volatilisation

Based on the vapour pressure of 0.07 hPa at 20ºC, cyclododecane is considered to be a volatile substance. Henry's law coefficient is calculated at > 100 Pa m^3 mol^{-1} (using vapour pressure mentioned above and all water solubility values given in Table 1) which indicates that the substance is highly volatile from water.

4.2.3 Long-range environmental transport

Cyclododecane is not subject to long-range atmospheric transport due to its short half-life in air.

4.3 Bioaccumulation (B)

4.3.1 Screening data[2]

BCFWIN v2.15 predicts BCF of 10,330 based on logK_{ow} of 6.12.

---

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

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

4.3.2 Measured bioaccumulation data[3]

Bioaccumulation of cyclododecane was studied in 1982 with common carp (*Cyprinus carpio*) (MITI, 1992). Nominal test concentrations of 3 and 30 µg l^{-1} were used. Tests were performed in a flow through system with 100 l glass tanks and with a flow rate of 1,155 l day^{-1}. Two dispersants (HCO-20 and HCO-40) were used in a concentration of 600 µg l^{-1} for each dispersant at the 30 µg l^{-1} test substance level and in a concentration of 60 µg l^{-1} at the 3 µg l^{-1} test substance level. Mean fish weight was 32.5 g and mean length 11 cm. Analysis of cyclododecane in water and fish were performed after 1, 2, 4, 6, 8 and 10 weeks. Two fish were sacrificed at each sampling occasion. Steady state appears to have been reached after 6 weeks based on measured concentrations in fish and water. A mean test concentration of 13 µg l^{-1} and a mean test concentration of 1 µg l^{-1} were measured corresponding to 30 µg l^{-1} and 3 µg l^{-1} nominal levels, respectively. Individual BCFs were calculated based on measured concentrations. The mean BCF of individual BCFs of the 6-10 week-samples was approximately 13,700 (wet weight basis) at both test concentrations. This value is considered to represent the steady state BCF. Despite of several weaknesses (use of dispersants, significant difference in nominal and measured concentrations and large variation of the results), this study is considered to give sufficient evidence on a very high bioaccumulation.

4.3.3 Other supporting information[4]

No data available.

4.3.4 Summary and discussion of bioaccumulation

For fish a BCF of 13,700 has been measured. The available QSAR-prediction is in line with the experimental result. It is concluded that cyclododecane has a very high bioaccumulation potential.

5 HUMAN HEALTH HAZARD ASSESSMENT

Data not reviewed for this report.

6 ENVIRONMENTAL HAZARD ASSESSMENT

6.1 Aquatic compartment (including sediment)

6.1.1 Toxicity test results

It should be noted that due to the high volatility of cyclododecane from aqueous solution, monitoring of test concentrations is crucial for the plausibility of the data.

---

[3] For example, fish bioconcentration factor

[4] For example, measured concentrations in biota

6.1.1.1 Fish

Acute toxicity

Hüls AG (1997) tested effects of cyclododecane on *Cyprinus carpio* in a semi static test according to the C.1. test guideline of Directive 84/449/EEC. The test solution was changed daily and test concentration was measured after and before the change of water (measured concentrations not reported in the IUCLID, Degussa AG, 2002). Test concentration was 1 mg l^{-1} which was the highest soluble concentration achieved. Temperature was 19.6-22.1ºC, dissolved oxygen stayed at 93-100% of saturation and pH was 8.0-8.6 during the test. One batch of ten fishes was used for the test and one fish was found dead at the day 4. LC_{50} (96 hours) > 1 mg l^{-1} resulted. It is noted that the Rapporteur did not evaluate the study as the report was not available.

MITI (1992) found LC_{50} (48 hours) of 21.8 mg l^{-1} for *Oryzias latipes* in a test according to the Japanese standard JISK-0102-1986-71. Test conditions are provided for the whole set of substances tested as follows. Test system was static or semi-static (not specified); temperature 25 ± 2ºC and 10 fish per concentration were used. Test concentrations were not obviously monitored and therefore the result is considered as not valid.

In a static 48-hour test according to DIN 38412 Teil 15 no effects were observed in *Leucidus idus* up to the water solubility limit (Huels-Untersuchung, unveröffentlicht). No monitoring of test concentrations occurred according to the IUCLID (European Commission, 2000) and the test is therefore considered as not valid.

Ecosar v0.99h predicts using the neutral organics QSAR without corrections LC_{50} (96 hours) of 0.017 mg l^{-1} for fish. The result is in contradiction with the test data above.

Long-term toxicity

No data available.

6.1.1.2 Aquatic invertebrates

Acute toxicity

A static study of Passino and Smith (1987) using *Daphnia pulex* resulted EC_{50} (48 hours) of 21 mg l^{-1}. Authors used ASTM procedures for the test. Five test concentrations were employed and solubility problems were encountered at higher test concentrations. Authors did not follow actual concentrations by monitoring. Hence, this test is considered not valid.

Hüls AG (1988) reported EC_{50} (24 hours) ≥ 2.6 mg l^{-1} for *Daphnia magna* from a DIN 38412 Teil 11 test. This study was not evaluated by the Rapporteur as the report was not available.

Ecosar v0.99h predicts LC_{50} (48 hours) of 0.024 mg l^{-1} for Daphnia. This result is in contradiction with the test data above.

Long-term toxicity

No data available.

6.1.1.3 Algae and aquatic plants

No effects were observed up to the highest test concentration (2.1 mg l^{-1}) in a test according to Directive 87/302/EEC, part C, p. 89 "Algal inhibition test" using *Scenedesmus subspicatus* (test duration 48 hours, static). Monitoring of test concentration was limited to the stock solution only (as cited in IUCLID of Degussa, 2002). Due to the volatility of cyclododecane its concentration in test vessels should have been monitored and the study is thus considered as not valid. It is noted that the Rapporteur could not fully evaluate the study as the report was not available.

Ecosar v0.99h predicts LC_{50} (72 hours) of 0.019 mg l^{-1} for algae. This result is in contradiction with the test data above.

6.1.2 Sediment organisms

No data available.

6.1.3 Other aquatic organisms

No data available.

6.2 Terrestrial compartment

No data available.

6.3 Atmospheric compartment

No data available.

7 PBT AND vPvB

7.1 PBT, vPvB assessment

Persistence: based on the biodegradability screening tests available, cyclododecane is considered to be not readily biodegradable. The substance has been observed to be degraded by adapted marine sediment micro-organisms and by specific microbial strains but no environmentally relevant degradation rates have been determined. The substance is therefore considered to meet the P/vP screening criterion. Further testing would be needed to quantify the rate of biodegradation in the environment, but based on the very slow or negligible biodegradation in the tests conducted with non-adapted organisms; it is considered that further information would be unlikely to give evidence on fast degradation. The substance is mainly used as intermediate, and it is therefore considered that no further testing is required at the present.

Bioaccumulation: the available study provides a BCF of 13,700 for fish. Cyclododecane is considered fulfilling the vB criterion.

Toxicity: QSARs predict acute $L(E)C_{50}$ values which are clearly below 0.1 mg l^{-1}. Of the data provided in the IUCLIDs, one fish test seems reliable providing $LC_{50} > 1$ mg l^{-1}. This study could not be evaluated by the Rapporteur as the report was not available. Other ecotoxicity results have

been reported, but due to lacking information on actual test concentrations, they are considered unreliable. In the absence of reliable toxicity data, cyclododecane is considered fulfilling the T screening criterion based on the QSAR predictions.

Summary: cyclododecane meets the vB criterion. The screening criteria for P/vP and T are also met. No further testing is proposed because the substance is used mainly as intermediate. The substance is concluded to be a PBT/vPvB substance based on the screening criteria.

INFORMATION ON USE AND EXPOSURE

Data not reviewed for the PBT-assessment.

OTHER INFORMATION

The following documents were mainly used as the source information and they contain the most references cited:

European Commission (2000) IUCLID Dataset, cyclododecane, CAS 294-62-2, 18.2.2000.

Degussa AG (2002) IUCLID Dataset, cyclododecane, CAS 294-62-2, 16.7.2002.

Other sources:

Hangleiter GmbH (2006) Cyclododecan. www.cyclododecane.net, 8.12.2006.

Kremer Pigments (2006) Homepage of Kermer Pigments GmbH. http://www.kremer-pigmente.de, 8.12.2006.

MITI (1992) Data on existing chemicals based on the CSCL Japan. Japan Chemical Industry Ecology-Toxicology & Information Center, 1992.