Substance name: Cyclododecane

EC number: 206-033-9

CAS number: 294-62-2

MEMBER STATE COMMITTEE SUPPORT DOCUMENT FOR AGREEMENT ON CYCLODODECANE

Adopted on 8 October 2008

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TABLES

Substance name: Cyclododecane

EC number: 206-33-9

CAS number: 294-62-2

It is considered that it is currently not possible to justify the identification of Cyclododecane as a substance of very high concern under Article 57 of REACH Regulation.

Summary of the evaluation:

The B and vB criteria under Annex XIII are met. However, only screening data are available for T and P

Therefore, there is currently not sufficient information available to conclude that cyclododecane can be identified:

- as a PBT/vPvB substance in accordance with Article 57(d) or (e) or
- as a substance of equivalent level of concern as specified in Article 57 (f).

JUSTIFICATION

1 IDENTITY OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

1.1 Name and other identifiers of the substance

Chemical Name: Cyclododecane

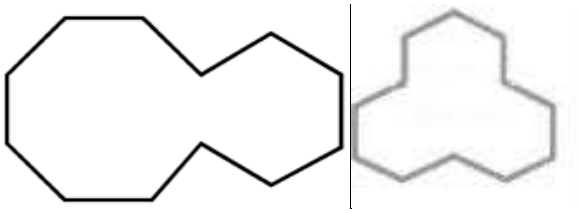
EC Name: 206-033-9

CAS Number: 294-62-2

IUPAC Name: Not relevant

Molecular Formula: C12H24

Structural Formula:



Molecular Weight: 168.33

1.2 Composition of the substance

Typical concentration (% w/w): Unknown

Concentration range (% w/w): Unknown

no relevant impurities

1.3 Physico-chemical properties

Table 1: Summary of physico-chemical properties (European Commission, 2000)

REACH ref Annex, §	Property	IUCLID section	Value	References
VII, 7.1	Physical state at 20°C and 101.3 kPa	4.1	solid	
VII, 7.2	Melting/freezing point	4.2	61°C	Hüls AG (1979). Study not evaluated
VII, 7.3	Boiling point	4.3	244°C at 1013hPa	Meyer and Hotz (1976). Study not evaluated
VII, 7.5	Vapour pressure	4.6	0.07 hPa at 20°c	Meyer and Hotz (1976). Study not evaluated
VII, 7.7	Water solubility	4.8	< 1 mg/l 10 mg/l 0.11 mg/l	MITI (1992) Sicherheitsdatenblatt Huels AG. Study not evaluated WSKOW v1.41
VII, 7.8	Partition coefficient n-octanol/water (log value)	4.7 partition coefficient	6.19 6.12 (calculated) 6.7 (calculated)	MITI (1992) KOWWIN v1.67 CLOGP3 by Huels AG Marl
XI, 7.16	Dissociation constant	4.21	Not available	

2 CLASSIFICATION AND LABELLING

2.1 Classification in Annex I of Directive 67/548/EEC

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

The substance was considered as a PBT/vPvB substance on the basis of screening criteria by the TC NES subgroup on identification of PBT and vPvB substances (EC, 2007).

2.2 Self classification(s)

No self classification

3 ENVIRONMENTAL FATE PROPERTIES

Cyclododecane may be released to the environment in wastewater streams, fugitive emissions generated at sites of its industrial production and sites of its use (Hall Howard, 1997). If released to soil, it is not expected to leach based upon an estimated Koc of 6500. If released to water, it may volatilize and partition to sediment.

3.1 Degradation

3.1.1 Stability

If released to the atmosphere, cyclododecane will abiotically be degraded. The rate constant for the vapour-phase reaction of cyclododecane with photochemically produced hydroxyl radicals has been estimated to be $1{,}67.10^{-11}$ cm^3/molecule-sec at 25°C, wich corresponds to an atmospheric half-life of about 23hr and a atmospheric concentration of 5.10^5 hydroxyl radicals par cm^3 (Atkinson, 1987).
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.
Alkanes are generally resistant to aqueous environmental hydrolysis (Lyman et al, 1990); therefore, cyclododecane is not expected to hydrolyze in the environment.

3.1.2 Biodegradation

3.1.2.1 Biodegradation estimation

No data available

3.1.2.2 Screening tests

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 of the TC NES subgroup on identification of PBT and vPvB substances 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 day**s 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.

3.1.2.3 Simulation tests

No data available

3.1.3 Summary and discussion of persistence

Very slow or no biodegradation at all was observed in the tests, even if a significant degradation has been shown by an adapted inocula with mixed microbial population and by specific strains. Cyclododecane is considered not readily biodegradable. It is not expected to hydrolyse abiotically in the environment.
Further information is needed to conclude if the substance is persistent in the environment.

3.2 Environmental distribution

3.2.1 Adsorption/desorption

Based on an estimated Koc value of 6500, cyclododecane may partition form the water column to sediment and suspended material (Sabljic, 1987). According to an estimated Koc value of 6500 (Sabljic, 1987), cyclododecane is expected to be relatively immobile in soil.

Insufficient data are available.

3.2.2 Volatilisation

Based on vapour pressure of 0.07 hPa at 20°C, cyclododecane is considered to be a volatile substance and expected to exist almost entirely in vapour-phase in the ambient atmosphere (Eisenreich et al., 1981). 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 and quickly volatile from water.
From water, volatilization half-lives of 3.8 and 45hr can be estimated for a model river (1m deep) and model pond (2m deep) respectively, when the effects of adsorption are not present (Lyman et al, 1990). In presence of adsorption (Koc of 6500), the volatilization half-life from the pond decreases to 43 days (EPA, 1987).

3.2.3 Distribution modelling

Cyclododecane is expected to exist almost entirely in vapour-phase in the ambient atmosphere (Eisenreich et al., 1981).

Cyclododecane is not subject to long-range atmospheric transport due to its short half-life in air. But adsorption to sediment in water may be important transport processes for cyclododecane.

Cyclododecane has been detected in all five of the great American lakes (Erie, Ontario, Huron, Superior and Michigan) aquatic ecosystems (Greta lakes water quality board, 1983) but concentrations, sampling dates and sample types were not reported by the authors.

No distribution modelling (e.g. Mackay level I) was performed.

3.3 Bioaccumulation

3.3.1 Aquatic bioaccumulation

3.3.1.1 Bioaccumulation estimation

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

An estimated BCF of 74.000 indicates that bioconcentration in aquatic organisms may be important (Lyman et al, 1990).

3.3.1.2 Measured bioaccumulation data

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 3µg 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 1µg l^{-1} were measured corresponding to 30 µg l^{-1} and 3µg 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.

3.3.2 Terrestrial bioaccumulation

No data available

3.3.3 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 and fulfils the B and vB criteria**.

3.4 Secondary poisoning

No data available

4 ENVIRONMENTAL HAZARD ASSESSMENT

4.1 Aquatic compartment (including sediment)

4.1.1 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.

4.1.1.1 Fish

Short-term toxicity to fish

Hüls AG (1997) tested effects of cyclododecane on *Cyprinus carpio* in a semi static test according to the C.1. test guideline of Directive 92/69/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 control fish was found dead at the day 4. LC_{50} (96 hours) > 1 mg l^{-1} resulted. It is noted that the rapporteur in the TC NES subgroup on identification of PBT and vPvB substances 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 LC50 (96 hours) of 0.017 mg l^{-1} for fish. The result is in contradiction with the test data above.

Long-term toxicity to fish

No data available

4.1.1.2 Aquatic invertebrates

Short-term toxicity to aquatic invertebrates

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 reporter 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 to aquatic invertebrates

No data available

4.1.1.3 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 92/69/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 of the TC NES subgroup on identification of PBT and vPvB substances 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.

5 PBT, VPVB AND EQUIVALENT LEVEL OF CONCERN ASSESSMENT

5.1 Comparison with criteria from Annex XIII

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. Cyclododecane is not expected to hydrolyse abiotically in the environment. The substance is therefore considered to meet the P/vP screening criterion according to the Guidance on Information requirements and Chemical safety assessment.

Further testing would be needed to quantify the rate of biodegradation in the environment and to conclude whether it fulfils the criteria for persistency according to Annex XIII.

Bioaccumulation: the available study provides a BCF of 13,700 for fish. Cyclododecane is considered fulfilling the B and vB criteria according to Annex XIII.

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 reporter 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.
As a consequence further information is needed in order to conclude whether the substance fulfils the criteria for toxicity according to Annex XIII.

5.2 Conclusion of PBT and vPvB or equivalent level of concern assessment

The B and vB criteria under Annex XIII are met. However, only screening data are available for T and P

Therefore, there is currently not sufficient information available to conclude that cyclododecane can be identified:

- as a PBT/vPvB substance in accordance with Article 57(d) or (e) or
- as a substance of equivalent level of concern as specified in Article 57 (f).

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