

## TC NES SUBGROUP ON IDENTIFICATION OF PBT AND VPVB SUBSTANCES

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

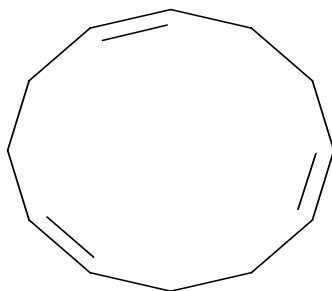
**Substance name:** Cyclododeca-1,5,9-triene

**EC number:** 225-533-8

**CAS number:** 4904-61-4

**Molecular formula:** C<sub>12</sub>H<sub>18</sub>

**Structural formula:**



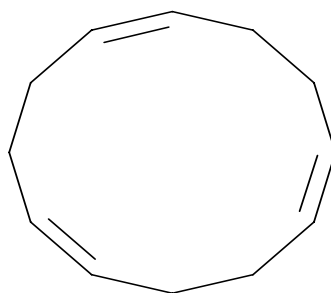
#### Summary of the evaluation:

Cyclododeca-1,5,9-triene is not considered to be a PBT –substance. It does not meet the P/vP-criteria based on screening data. It fulfils the vB –criterion. The assessment of ecotoxicity was not finalised.

## JUSTIFICATION

### 1 IDENTIFICATION OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

Name: Cyclododeca-1,5,9-triene  
 EC Number: 225-533-8  
 CAS Number: 4904-61-4  
 IUPAC Name:  
 Molecular Formula: C<sub>12</sub>H<sub>18</sub>  
 Structural Formula:



Molecular Weight: 162.28  
 Synonyms: 1,5,9-Cyclododecatriene  
 1,5,9-Cyclododecatriene (6CI, 8CI, 9CI)  
 CDT (abbrev.)

#### 1.1 Purity/Impurities/Additives

No data available.

#### 1.2 Physico-Chemical properties

Table 1 Summary of physico-chemical properties. For details and references, see European Commission (2000) . Data provided have not been evaluated by the Rapporteur.

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	-17 °C -18 °C	Shell Chemicals (1993) Huels AG (1994)
VII, 7.3	Boiling point	227 °C 237 °C at 1013 hPa	Shell Chemicals (1993) Huels AG (1994)
VII, 7.5	Vapour pressure	Ca 0.12 hPa at 20 °C 1.3 hPa at 50 °C	Extrapolation, Huels AG (1994) Shell Chemicals (1993)
VII, 7.7	Water solubility	5.0 mg l <sup>-1</sup> at 25 °C 0.3898 mg l <sup>-1</sup> at 25 °C	Huels AG (1994) Estimate (WSKOW v1.41)
VII, 7.8	Partition coefficient n-octanol/water (log value)	5.48	Calculated (KOWWIN v1.67)

		4.1 at 25 °C 4.5 at 23 °C 5.076 5.65 5.77 6.8	Bennet, D. and Bryant, K. (1982) Huels study (1989) Calculated (CLOG3) Comparable to OECD 117 (McDuffie, 1981; as cited in Degussa AG, 2002) Comparable to OECD 117 (Eadsforth and Moser, 1983; as cited in Degussa AG, 2002) EPA/600/S-96/005 (slow stirring method) (Wo, 2002; as cited in Degussa AG, 2002)
	Dissociation constant	-	

## 2 MANUFACTURE AND USES

Nine producers/importers have provided information under Regulation 93/793/EEC.

According to European Commission (2000), the substance is used in closed systems as well as in a non-dispersive or wide dispersive manner. Listed uses are:

- additive in construction materials
- fillers
- insulating materials
- intermediates
- reinforcing resin for styrene-butadiene rubbers
- stabilizer and plasticizer for thermoplastic polymers.

The substance is used in quantities between 50 000 – 100 000 tonnes per year (European Commission, 2000).

Based on more recent information from industry CDT is solely used as intermediate in chemical synthesis (Degussa AG, 2002).

## 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

Indirect photochemical degradation in the atmosphere is considered to be fast based on the estimated half-life of 2.2 hours for the reaction with OH-radicals using AOP v1.91 (24 h day<sup>-1</sup>; 5\*10<sup>5</sup> OH<sup>-</sup> cm<sup>-3</sup>).

#### 4.1.2 Biotic degradation

Davis et al. (2006a) employed t,t,t1,5,9-cyclododecatriene in a ready biodegradability test according to OECD 301F at test concentrations of 1 and 10 mg l<sup>-1</sup>. CDT was dispersed into the test medium by coating it onto silica gel (mixing on a roller bank for 72 h; loadings of 1 and 10 mg CDT/g silica gel used). The incubation with an inoculum of activated sludge from Midland municipal waste water treatment plant, Michigan, U.S. was carried out in 160 ml glass serum bottles with a nominal 85 ml headspace at 20±2 °C in the dark on a rotary shaker for 60 days. Final concentration of the inoculum was 30 mg SS l<sup>-1</sup>. CDT was analysed with HPLC-UV (and GC-UV) at frequent intervals from triplicate reaction mixtures. A parallel set of vials were used to analyse CO<sub>2</sub>-evolution.

CDT started to disappear at both test concentrations after a lag phase of at least 14 days. No significant CO<sub>2</sub>-production took place during the test compared to controls. No significant disappearance was observed in the autoclaved sterile controls and water controls indicating, that disappearance in the viable flasks was caused by biodegradation and no significant losses via volatilisation, adsorption or abiotic degradation occurred. Results during the course of the study are presented in Table 4.1. At 10 mg l<sup>-1</sup> test level CDT disappeared slightly more slowly than at the lower test concentration. This may have been caused by a slight inhibition (aniline+CDT used for inhibition control). Due to a high variability in the CO<sub>2</sub>-respiration in the test, no firm conclusion could be made on the potential mineralisation of CDT. The study is well documented and results are considered reliable. The results indicate, that although CDT is not readily biodegradable, it is subject to a relatively fast biodegradation.

Table 4.1. Biodegradation results (as % remaining of initial concentration) in the study of Davis et al. (2006a).

Test concentration	Day				
	14	21	28	42	60
1mg l <sup>-1</sup>	86	72	55	<7	na
10 mg l <sup>-1</sup>	93	82	79	57	38

Davis et al. (2006b) used essentially similar experimental conditions as Davis et al. (2006a) (although OECD 301B as the underlying procedure) but applied test concentrations of 0.2 mg l<sup>-1</sup> and 1 mg l<sup>-1</sup> and used <sup>14</sup>C-labelled CDT (ring labelled at 6 carbons). The disappearance of CDT was monitored by HPLC-RCD and the ultimate degradation was followed by means of <sup>14</sup>CO<sub>2</sub>-analysis. Duplicate test vials were sampled at frequent intervals. Results during the course of the test are presented in Table 4.2. After 63 (77) days of incubation, the <sup>14</sup>CO<sub>2</sub> formation reached ca. 50 (70) % at 0.2 (1) mg l<sup>-1</sup> test concentration, respectively. A phase of slow mineralisation until ca. 35 days (44.5 % CDT remaining; 11 % of CDT mineralised at 0.2 mg l<sup>-1</sup> level) was observed. Recovery of <sup>14</sup>CDT in abiotic controls was 96 % on day 63 (lower exposure level) and 97 % on day 77 (higher exposure level) indicating, that no losses other than biodegradation took place.

Table 4.2 *t,t,t-<sup>14</sup>C*/CDT and <sup>14</sup>CO<sub>2</sub> concentrations at different sampling times (percent of Day 0)

Test conc. (mg l <sup>-1</sup> )		Day							
		7	14 (15)*	21	28	35	49 (50)*	63	77
0.2	CDT remaining	80.8±5.4	74.1±1.3	65.3±2.8	39.0±27.7	44.5±3.1	27.7±33.5	8.3±6.1	-

	CO <sub>2</sub> formed	Nd <sup>a</sup>	3.4±0.2	5.6 ± 0.1	8.1±1.8	11.1±1.2	31.2±16.1	49.7±9.6	–
1	CDT remaining	86.3±0.1	80.8±8.0	77.0±4.7	82.6± 5.1	74.0±8.4	34.3±47.4	44.5±29.9	Nd
	CO <sub>2</sub> formed	Nd	4.5±1.7	5.5 ± 1.2	8.1±1.0	–	17.6±8.3	31.6±10.6	68.2±3.0

<sup>a</sup> sampling day for CO<sub>2</sub> in parenthesis

<sup>a</sup> not detected – Approximate detection limit (3 x signal/noise) was 4% of initial radioactivity for 0.2 mg l<sup>-1</sup> t,t,t-[<sup>14</sup>C]CDT test mixtures and 0.8% of initial radioactivity for 1 mg l<sup>-1</sup> t,t,t-[<sup>14</sup>C]CDT test mixtures

<sup>b</sup> not analyzed

<sup>c</sup> Average of duplicate samples ± 1 Standard Deviation

During the study of Davis et al. (2006b), a transient degradation product with a shorter elution time than CDT was detected by HPLC-analysis. The peak size of this (unidentified) product increased during the first month and decreased towards the end of the study. The study is well documented and the results are considered plausible. Based on the results, CDT is considered to be not readily biodegradable, but due to the extent of mineralisation reached, the substance can be expected to be not persistent.

MITI (1992) has reported on a ready biodegradability test (modified MITI-method), where 0 % was degraded in 14 days. The report was not available to the Rapporteur for evaluation. Huels AG (as cited in European Commission, 2000; study report not available to the Rapporteur) observed that 0 % was degraded in 28 days in an OECD 301D –test.

In another ready biodegradability test according to OECD 301D, 1 % of CDT was observed to have degraded after 28 days (DuPont Co., 2000 as cited in Degussa, 2002). It is noted, that the study report was not available to the Rapporteur for evaluation.

Two additional biodegradation screening studies are available. The first study (Hamwijk and Cremers, 2005a) was inconclusive as the test substance (c,t,t-CDT) was inadequately dosed to the test system. In this study CDT, dissolved in hexane, was applied to filter paper which after evaporation of the hexane was added to the test medium. It appeared that CDT had evaporated from the filter paper together with the hexane before it was added to the test medium.

In the second study (Hamwijk, 2005b) t,t,t-CDT, was added directly to the filter paper to circumvent the problem of evaporation. Analytical measurements confirmed that the test substance was adequately dosed. No mineralisation was observed and a recovery of 84-113% of the nominal dose after 28 d of incubation indicated that no primary degradation had occurred. The test substance appeared to remain on the filter as a small clot and the authors speculate that the absence of degradation may have been caused by a small surface area of the substance on the filters, thus reducing the bioavailability.

#### 4.1.3 Other information <sup>1</sup>

CDT is the main degradation product of hexabromocyclododecane (HBCDD; CAS 25637-99-4). Data on HBCDD have been presented in the PBT summary no. 58. Despite the fact, that primary degradation and even mineralisation was observed in the two reliable screening tests with CDT, no mineralisation was observed in the simulation and screening degradation studies with HBCDD. This is likely to be caused by two facts. Firstly, the duration of HBCDD-experiments could not be

<sup>1</sup> For example, half life from field studies or monitoring data

long enough to discover any mineralisation even in those favourable conditions, where HBCDD was degraded in relevant amounts to CDT. Secondly, significant degradation of HBCDD to CDT was observed only in anaerobic conditions, whereas it is likely, that further degradation of CDT would need aerobic conditions. Hence, the available degradation data on HBCDD cannot be directly used to judge on the overall degradation potential of CDT in the environment and vice versa.

#### **4.1.4 Summary and discussion of persistence**

The available experimental screening biodegradation data indicate that CDT is not readily biodegradable. Despite of this, 50 (70) % of the test concentration was observed to be mineralized after 63 (77) days in enhanced ready biodegradation test (OECD 301B) conditions (Davis et al., 2006b) and therefore CDT it is not considered to be persistent. The conclusion is supported by results of a similar enhanced test of Davis et al. (2006b) modified from OECD 301F. In this study, primary degradation of CDT was complete after 42 days at the lower exposure level (= CDT not detected) and 38 % of CDT was remaining after 60 days at the higher exposure level. It must be noted, that it is likely, that the ready biodegradability tests not evaluated by the Rapporteur have had problems with volatilisation losses or the test concentrations have caused inhibition.

CDT is an anaerobic degradation product of hexabromocyclododecane (CAS 25637-99-4). Data on this substance have been presented in the PBT summary no. 58. Nevertheless, the available degradation data on HBCDD cannot be directly used to judge on the overall degradation potential of CDT in the environment and vice versa. Firstly, the duration of biodegradation tests were not long enough to discover any mineralisation even in those favourable conditions, where HBCDD was degraded in relevant amounts to CDT. Secondly, significant degradation of HBCDD to CDT was observed only in anaerobic conditions, whereas it is likely, that further degradation of CDT in the environment would need aerobic conditions (tests only available for aerobic conditions).

## **4.2 Environmental distribution**

### **4.2.1 Adsorption**

### **4.2.2 Volatilisation**

### **4.2.3 Long-range environmental transport**

## **4.3 Bioaccumulation (B)**

### **4.3.1 Screening data**

A logKow of 5.48 has been estimated by KOWWIN v1.67. Measured logKow –values between 5.65 and 6.8 are also available.

### 4.3.2 Measured bioaccumulation data

MITI (1992) has reported on an OECD 305C flow-through bioconcentration test with *Cyprinus carpio*. Based on further information from CITI (2003), dispersants HCO-20 and HCO-40 were used in concentrations of 250 µg l<sup>-1</sup> and 25 µg l<sup>-1</sup> for two exposure levels, respectively. The measured exposure concentrations were during the test ca. 5.5-7.0 µg l<sup>-1</sup> (Level 1; 10 µg l<sup>-1</sup> nominal) and 0.44-0.67 µg l<sup>-1</sup> (Level 2; 1 µg l<sup>-1</sup> nominal). BCFs of all sampling occasions for each fish as calculated from measured data in fish and water are presented in Table 4.3.

Table 4.3 BCF –values for *Cyprinus carpio* during the 10 weeks exposure period (CITI, 2003).

Level	1 weeks	2 weeks	4 weeks	6 weeks	8 weeks	10 weeks
1	2 690	5 140	4 840	12 500	9 750	5 560
	3 370	2 630	8 070	10 800	8 850	8 960
2	1 920	4 590	4 080	5 610	9 270	10 300
	2 950	2 450	3 240	4 830	14 800	6 220

It seems that steady state was reached during the exposure period and despite the use of dispersants, the test concentrations have been adequately low to be below the limit of water solubility. Based on the calculation of the Rapporteur, a mean BCF of all results was  $6\,930 \pm 3\,326$  and “steady-state” BCF (mean of 6-10 weeks)  $9\,403 \pm 2\,321$  for the higher exposure level. Corresponding values for the lower exposure level were  $5\,855 \pm 3\,811$  (overall mean BCF) and  $10\,147.5 \pm 3\,553$  (“steady-state” BCF). The results are considered reliable enough for the purpose of this assessment.

### 4.3.3 Other supporting information<sup>2</sup>

In a recent study, bird eggs from remote islands in northern Norway were analysed for brominated flame retardants and CDT (Knudsen et al, 2005). CDT was below the detection limit (0.5 µg kg<sup>-1</sup> ww) in all samples. Nevertheless, the authors noted, that the quality of the analytical method could not be assured.

### 4.3.4 Summary and discussion of bioaccumulation

Reliable experimental BCFs are available from an OECD 305C –test with *Cyprinus carpio*. A mean BCF during the course of the 10 weeks test was  $6\,930 \pm 3\,326$  (higher exposure level) and  $5\,855 \pm 3\,811$  (lower exposure level) and corresponding steady-state BCFs  $9\,403 \pm 2\,321$  and  $10\,147.5 \pm 3\,553$ . It is concluded that the substances has a very high bioaccumulation potential.

## 5 HUMAN HEALTH HAZARD ASSESSMENT

Data not reviewed for this report.

<sup>2</sup>For example, measured concentrations in biota

## **6 ENVIRONMENTAL HAZARD ASSESSMENT**

### **6.1 Aquatic compartment (including sediment)**

Acute ecotoxicity data are available for CDT. Due to the high volatility and low water solubility of CDT, tests without test substance monitoring cannot be considered to be reliable. It is noted that even in flow-through conditions of the BCF-test (see section 4.3.2) the measured exposure concentrations were ca. 45-70 % of the nominal concentrations. Ecotoxicity test reports were not available to the Rapporteur for evaluation and therefore it is not possible to evaluate the plausibility of the available results.

#### **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

**Persistence:** Cyclododeca-1,5,9-triene (CDT) does not meet the P/vP criteria according to screening data. Based on two reliable enhanced tests on ready biodegradability (OECD 301F and 301B), the substance is not readily biodegradable. Due to the extent of primary degradation observed in both tests and due to the fact that mineralisation followed in one of the two tests reached 50 (70) % of the initial test concentration after 63 (77) days, it is considered, that CDT is not persistent in the sense of the PBT -criteria.

**Bioaccumulation:** CDT fulfils the vB criterion. In a reliable standard OECD 305C test with *Cyprinus carpio*, a mean BCF during the course of the 10 weeks test was  $6\,930 \pm 3\,326$  (higher exposure level) and  $5\,855 \pm 3\,811$  (lower exposure level) and corresponding steady-state BCFs  $9\,403 \pm 2\,321$  and  $10\,147.5 \pm 3\,553$ .

**Toxicity:** Assessment of ecotoxicity was not completed.

**Summary:** Cyclododeca-1,5,9-triene does not meet the P/vP-criteria based on screening data but it fulfils the vB –criterion. The assessment of ecotoxicity was not completed. It is concluded, that cyclododeca-1,5,9-triene 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 source:

European Commission, 2000. IUCLID Dataset, Cyclododeca-1,5,9-triene, CAS 4904-61-4, 18.2.2000.

Other sources:

CITI, 2003. Additional information on the METI –tests provided to ECB on 7.10.2003.

Davis, J., Gonsior, S., and Hales, C., 2006a. The aerobic biodegradability of trans, trans, trans-1, 5, 9-Cyclododecatriene in a modified ready biodegradation test. Toxicology & Environmental Research and Consulting, The Dow Chemical Company, Michigan. Sponsor: European Brominated Fire Retardant Industry Panel. Study ID: 051165.

Davis, J., Gonsior, S., Hales C., 2006b. The aerobic biodegradability of trans, trans, trans-1, 5, 9-[14C]Cyclododecatriene in a modified ready biodegradation test. Toxicology & Environmental Research and Consulting, The Dow Chemical Company, Michigan. Sponsor: European Brominated Fire Retardant Industry Panel. Study ID: 061099.

Degussa AG, 2002. IUCLID Data Set, Cyclododeca-1,5,9-triene, CAS 4904-61-4, 18-SEP-2002.

Hamwijk M and Cremers R. Determination of the ready biodegradation of 1, 5, 9-Cyclododecatriene (CAS# 4904-61-4) in a Closed Bottle Test (OECD Guideline No. 301D, EU C.4-E). 2005a; TNO Report V6395.

Hamwijk M and Cremers RKH. Determination of the ready biodegradability of t,t,t-1,5,9-Cyclododecatriene (CAS# 676-22-2) in a Closed Bottle Test (OECD Guideline No. 301D, EU C.4-E). 2005b; TNO Report V6553/02.

Knudsen, L., Gabrielsen, G., Verreault, J., Barrett, R., Skåre, J., Polder, A. and Lie, E., 2005. Temporal trends of brominated flame retardants, cyclododecan-1,5,9-triene and mercury in eggs of four seabird species from Northern Norway and Svalbard. Statens forurensningtilsyn. SPFO-Report: 942-2005.

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.