TC NES SUBGROUP ON IDENTIFICATION OF PBT AND VPVP SUBSTANCES

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

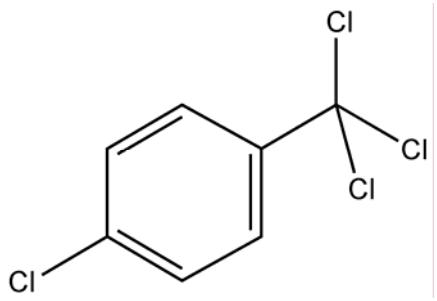
Substance name: α, α, α, 4-tetrachlorotoluene

EC number: 226-009-1

CAS number: 5216-25-1

Molecular formula: C7H4Cl4

Structural formula:



Summary of the evaluation:

α, α, α, 4-tetrachlorotoluene (4-CBT) is not considered to be a PBT substance. The substance does not meet the P criterion. It may fulfil the B/vB criteria according to screening data, but its bioaccumulation potential was not assessed further due to its fast hydrolysis. The hydrolysis product 4-chlorobenzoic acid (4-CBA) does not fulfil the P/vP and B/vB criteria based on screening data. The T criterion is fulfilled for 4-CBT for human health. Ecotoxicity of the substance was not assessed.

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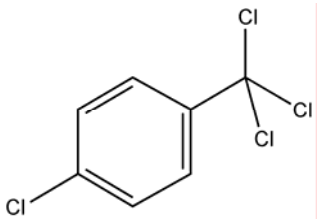
JUSTIFICATION

1 IDENTIFICATION OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

Name: α, α, α,4-tetrachlorotoluene
EC Number: 226-009-1
CAS Number: 5216-25-1
IUPAC Name:
Molecular Formula: C7H4Cl4
Structural Formula:



Molecular Weight: 229.92
Synonyms: p-Chlorobenzotrichloride; p-Trichloromethylchlorobenzene; 1-Chloro-4-(trichloromethyl)benzene; 4-Chlorobenzotrichloride; 4-CBT (for full list of synonyms, see European Commission, 2000)

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).

REACH ref Annex, §	Property	Value	Comments
V, 5.1	Physical state at 20 C and 101.3 Kpa	liquid	European Commission, 2000
V, 5.2	Melting / freezing point	4-5 ºC	Hoechst AG (1993 and 1997); data not evaluated
V, 5.3	Boiling point	240 ºC (at 1013 hPa)	Hoechst AG (1993 and 1997); data not evaluated
V, 5.5	Vapour pressure	0.04 hPa (at 20 ºC)	Hoechst AG (1993 and 1997); data not evaluated
V, 5.7	Water solubility	4.0 mg l^{-1} (calculated; at 25 ºC) 4-CBA (hydrolysis product): 387.1 mg l^{-1} (calculated; at 25 ºC) 72 mg l^{-1} (at 25 ºC)	WSKOW v1.41; the applicability of the model for the substance is questionable (*). WSKOW v1.41 . WSKOW v1.41 experimental database; data not evaluated
V, 5.8	Partition coefficient n-octanol/water (log value)	4.54 (calculated) 4.8 (calculated)	KOWWIN v1.67 ; the applicability of the model for the substance is questionable (*) CLOGP3; the applicability of the model for the substance is questionable
VII, 5.19	Dissociation constant		

(*) The experimental databases of EPISUITE programs do not contain substances from the group for chlorotoluenes. The substance is expected to react fast with nucleophiles like OH^-, N or S; a true water solubility or logKow of the substance is very difficult to determine.

2 MANUFACTURE AND USES

Three companies have notified the substance.

3 CLASSIFICATION AND LABELLING

Classification and labelling according to the Annex I of Directive 67/548/EEC:

Classification

Carc. Cat 2; R45	May cause cancer
Repr. Cat. 3; R62	Possible risk of impaired fertility
T; R48/23	Danger of serious damage to health by prolonged exposure through inhalation
Xn; R21/22	Harmful in contact with skin and if swallowed
Xi; R37/38	Irritating to respiratory system and skin

4 ENVIRONMENTAL FATE PROPERTIES

4.1 Degradation (P)

4.1.1 Abiotic degradation

Indirect photochemical degradation in the atmosphere is considered to be very slow based on the estimated half-life of 64 days for the reaction with OH-radicals using AOP v1.91 (24 h day^{-1}; $5*10^5$ OH^- cm^{-3}).

Dietz (1981) tested hydrolysis of α, α, α, 4-tetrachlorotoluene (4-CBT) in distilled, deionized water. The initial test concentration was 100 mg l^{-1}, which was according to the author above the water solubility of the substance. The test substance was therefore introduced to the test solution as (liquid-liquid) suspension. The high test concentration was needed according to the author to be able to follow analytically the decrease of concentration during the test. No pH buffer was used. Vials of 4 ml water volume were used for the test and the test substance was added to the vials in 40 µl stock solution (10 mg 4-CBT ml^{-1} water; prepared directly before the test). The solution was gently swirled during the test. An aliquot of the solution was directly injected into a HPLC for analysis. The initial test concentration was measured by injecting the stock solution to 4 ml acetonitrile from which an aliquot was sampled for analysis. Concentration of the substance was measured using HPLC (15 % H_2O:85 % MeOH as eluent) with UV-detector at 254 nm. Emergence of the final hydrolysis product 4-chlorobenzoic acid was according to the author observed simultaneously. The author mentions that the test was intended to provide approximate results (the system was not calibrated against the whole concentration range). Half-life for the substance was determined as T/3 (= three half-lives; the time where 87.5 % of the initial concentration had disappeared).

The anticipated reaction route of 4-CBT is illustrated in Figure 1. 4-CBT is hydrolysed first to 4-chlorobenzoyl chloride which reacts rapidly further to 4-chlorobenzoic acid. 3 moles of HCl are formed simultaneously leading to a decrease of pH in the test solution.

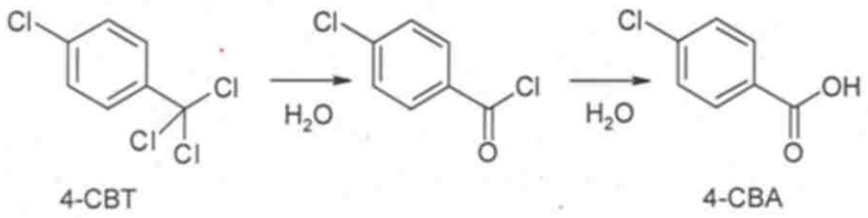


Figure 1. Hydrolysis products of 4-CBT.

Dietz (1981) found the following (apparent) half-lives at 0 ºC and 25 ºC:

	0 ºC	25 ºC
DT_{50} in water (min)	38	1.7

It must be noted that pH of the test at the start and during the test was not provided by the author. pH at the start can be assumed to be around 7 for deionized water. During hydrolysis of 4-CBT, pH decreases without buffer. As the reaction rate is depending on the concentration of nucleophiles (in this case OH^-), the rate of hydrolysis is decreasing with decreasing pH after the reaction has started. The test system has therefore measured the "worst case" hydrolysis rate regarding the influence of

pH (or regarding the availability of nucleophiles in environmental conditions). It must, however, be noted that decrease of pH is not allowed in standard hydrolysis test of Annex V of 67/548/EEC. In addition, the initial concentration was measured as dissolved to acetonitrile, which has probably dissolved 4-CBT completely, whereas in the test vials the reaction rate was regulated by the presence of phases (dissolution/mixing and hydrolysis). No information was provided at which point of time all suspended test substance had disappeared.

Due to the test conditions, the reported half-lives do not represent the actual hydrolysis half-life in water, but rather an apparent rate of disappearance which is influenced both by hydrolysis and dissolution in the test solution and potentially in the analysis equipment.

Despite the unclear kinetics and documentation deficits, it is obvious that hydrolysis has occurred in the test system in a very short period of time. In addition, simultaneous emergence of the hydrolysis product 4-CBA was mentioned by the author. Therefore it is considered, that the study can be used as an evidence of fast hydrolysis of 4-CBT in water.

Hoechst AG (1993) has reported that this substance hydrolyses whereas the rate is dependent on temperature. HCl was reported as the reaction product. The study was not available to the Rapporteur for evaluation.

Hydrolysis of a structurally similar substance α,α,α,-trichlorotoluene (CAS 98-07-7) has been tested at constant pH (at pH 5 and pH 7) by two authors resulting a hydrolysis half-life of few minutes (OECD, 2004).

4.1.2 Biotic degradation

Biodegradation data of 4-CBT was not reviewed for this report. Due to the fast hydrolysis, biodegradation of the parent compound is considered to be of secondary interest for the assessment of persistence.

For the hydrolysis product 4-CBA (CAS 74-11-3) following data are available:

Biodegradation	Result	Source
Biowin 1	Biodegrades fast (0.67)	Biowin v4.02
Biowin 2	Biodegrades fast (0.77)	
Biowin 3	Weeks-months (2.7)	
Biowin 4	Days-weeks (3.5)	
Biowin 5	Biodegrades fast (0.66)	
Biowin 6	Biodegrades fast (0.67	
Ready biodegradability prediction:	Not readily biodegradable	
Closed Bottle Test	Biodegrades fast	Bayer AG (1978/2002)

Bayer AG (1978) measured biodegradation of 4-CBA in a closed bottle test according to the draft OECD 301 D guidance. Test temperature was 20 º C and test concentration 2.4 mg l^{-1}. Higher test concentrations used (8, 24 and 80 mg l^{-1}) caused inhibition. Both adapted (14 days pre-exposure) and non-adapted inocula (10^3-10^6 cells l^{-1}) were employed. For the stock solution (1 g l^{-1}) an emulsifier (CAS 68130-72-3) was used. Phenol was tested as a reference substance. Biodegradation with non-adapted microorganisms was 0 % at day 5, 0 % at day 10 and 72.7 % at day 20 measured as BOD/ThOD. Biodegradation with adapted inoculum was 0 % at day 5, 81.8 % at day 10 and 92.9

% at day 20. The test is not fully documented according to the standard requirements and too few sampling occasions took place to confirm that a degradation plateau would have been achieved at day 20. Hence, the test is considered valid with restrictions. 4-CBA is considered readily biodegradable based on the results.

4.1.3 Other information [1]

Data not reviewed for this report.

4.1.4 Summary and discussion of persistence

It is concluded that the substance is not stabile in aqueous solution but undergoes a fast hydrolysis. The hydrolysis product 4-CBA is readily biodegradable based on a test according to (a former) draft OECD 305.

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[2]

Predicted BCFs from 625 to 991 (BCFWIN v2.15) were obtained using estimated logKow-values of 4.54 and 4.8, respectively. The Connell model (recommended by TGD) predicts a BCF at 3981 using a log Kow value of 4.54 . It must be noted, that the calculated logKow –values are not necessarily reliable due to the fast hydrolysis.

The hydrolysis product 4-CBA does not have high bioaccumulation potential based on the log Kow of 2.65 (Hansch, et al.,1995; from EPIWin v3.12 database).

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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]

No experimental data on bioaccumulation are available for 4-CBT and its hydrolysis product.

4.3.3 Other supporting information[4]

No data available.

4.3.4 Summary and discussion of bioaccumulation

No experimental data on bioaccumulation are available for 4-CBT and its hydrolysis product 4-CBA. Despite the high estimated logKow -values of 4-CBT (4.54 and 4.8), it is considered that it is not necessary to assess further its bioaccumulation potential. Due to the fast hydrolysis, exposure of the environment to the substance is unlikely or very low. Experimental logKow of the hydrolysis product 4-CBA is 2.65 indicating low to moderate bioaccumulation potential.

5 HUMAN HEALTH HAZARD ASSESSMENT

Data not reviewed for this report.

6 ENVIRONMENTAL HAZARD ASSESSMENT

Data not reviewed for this report.

[3] For example, fish bioconcentration factor

[4] For example, measured concentrations in biota

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

6.1.3 Other aquatic organisms

6.2 Terrestrial compartment

6.3 Atmospheric compartment

7 PBT AND vPvB

7.1 PBT, vPvB assessment

Persistence: 4-CBT does not fulfil the P criterion. The substance is not stabile in aqueous solution but undergoes a fast hydrolysis. The hydrolysis product is 4-CBA, which is readily biodegradable and hence does not fulfil the screening P/vP criteria.

Bioaccumulation: 4-CBT may fulfil the B/vB criteria based on screening data. No experimental data on bioaccumulation are available for 4-CBT and its hydrolysis product 4-CBA. Further testing of 4-CBT is not considered necessary due to the fast hydrolysis. LogKow of 4-CBA is 2.65 and hence it

does not fulfil B/vB criteria according to screening data. Toxicity: the substance is considered fulfilling the T criterion for human health due to the classification as carcinogenic, category 2.

Summary: 4-CBT does not meet the P criterion. It may meet the B/vB criteria according to screening data, but its bioaccumulation potential was not further assessed due to the fast hydrolysis. The hydrolysis product 4-CBA does not fulfil the P/vP and B/vB criteria based on screening data. The T criterion is fulfilled for human health due to the classification as Cat 1 carcinogenic substance. Ecotoxicity of 4-CBT was not assessed. It is concluded that the substance 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 mainly taken from the following sources:

European Commission, 2000. IUCLID Dataset, α, α, α, 4-tetrachlorotoluene, CAS 5216-25-1, 19.2.2000.

Other sources:

Bayer AG, 1978. Biodegradation, p-Chlorobenzoic acid. Unpublished investigation, study number 78/576, June 1978, Report: 2002-05-21.

Dietz, 1981. Unpublished investigation (4852-122-136) cited in EPA/OTS (1987): Doc No. 40-8715088, NTIS Order No. NTIS/OTS0526145 (TCSA Sect. 4 Submission from Occidental Chemical Corp 1987-07-27).

OECD, 2004. SIDS Initial Assessment Report for SIAM 18, Paris, France, 20-23 April, 2004. α,α,α,-trichlorotoluene (Trichloromethylbenzene), CAS 98-07-7. UNEP Publications.