TC NES SUBGROUP ON IDENTIFICATION OF PBT AND VPVP SUBSTANCES

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

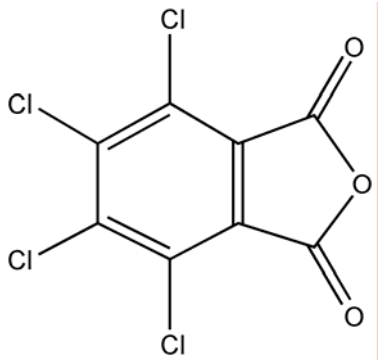
Substance name: Tetrachlorophthalic anhydride

EC number: 204-171-4

CAS number: 117-08-8

Molecular formula: C8Cl4O3

Structural formula:



Summary of the evaluation:

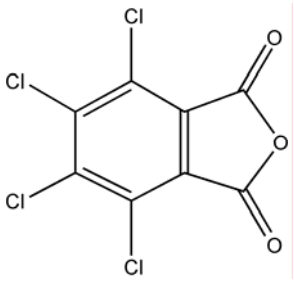
Pure tetrachlorophthalic anhydride is not considered to be a PBT substance. The pure substance does not meet the P criterion due to a fast hydrolysis. It meets the screening B criterion but its bioaccumulation potential was not assessed further due to the fast hydrolysis. The stable hydrolysis product tetrachlorophthalic acid (CAS 632-58-6) does not meet the screening B criterion. Ecotoxicity of tetrachlorophthalic anhydride or its hydrolysis product was not evaluated.

Commercial tetrachlorophthalic anhydride may contain a POP impurity (hexachlorobenzene, CAS 118-74-1). The presence and concentration of this impurity depends on the manufacturing process. Hexachlorobenzene is a persistent organic pollutant (POP) subject to Regulation 2004/850/EC.

JUSTIFICATION

1 IDENTIFICATION OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

Name: Tetrachlorophthalic anhydride
EC Number: 204-171-4
CAS Number: 117-08-8
IUPAC Name:
Molecular Formula: C8Cl4O3
Structural Formula:



Molecular Weight: 285.9
Synonyms: Phthalic anhydride, tetrachloro-; 1,3-Isobenzofurandione, 4,5,6,7-tetrachloro-; 1,3-Dioxo-4,5,6,7-tetrachloroisobenzofuran; tetrathal; 1,3-Isobenzofurandione, tetrachloro-

1.1 Purity/impurities/additives

One company has reported that hexachlorobenzene (CAS 118-74-1) is present in their commercially available tetrachlorophthalic anhydride as an impurity in a concentration of ≥ 0.1 - ≤ 0.5% (w/w). This company has ceased their production and import in the EU. Another company has confirmed, that hexachlorobenzene is present in a concentration of < 0.1% w/w in their product.

On the basis of the information available, it can be expected that hexachlorobenzene is present as an impurity in commercial tetrachlorophthalic anhydride products, but the concentration of the impurity varies from producer to producer.

Hexachlorobenzene is a persistent organic pollutant subject to Regulation 2004/850/EC as amended by Regulation 2006/1195/EC.

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	Solid	Solutia, Inc. (2002a)
V, 5.2	Melting / freezing point	254.5ºC	Weast (1979) as cited in Solutia, Inc. (2002a) (data not evaluated)
V, 5.3	Boiling point	371ºC	Hawley (1975) as cited Solutia, Inc. (2002a) (data not evaluated)
V, 5.5	Vapour pressure	0.21 hPa at 145ºC	Hawley (1975) as cited in Solutia, Inc. (2002a) (data not evaluated)
V, 5.7	Water solubility*	4 g l^{-1}* < 1 mg l^{-1} (at 21ºC)*	IPCS (1994) (data not evaluated) NTP Chemical Repository as cited in Solutia, Inc. (2002a) (data not evaluated)
V, 5.8	Partition coefficient n-octanol/water (log value)	4.65 3.57*	KOWWIN v1.67 Solutia, Inc.*, (2002a) (data not evaluated)
VII, 5.19	Dissociation constant		

* It is noted that it is not clear for which form of the substance (parent compound or hydrolysis product) the water solubility and logKow value has been reported.

2 MANUFACTURE AND USES

Four companies have notified the substance. The substance is listed as a LPV –chemical on the basis of the data collection under Regulation 93/793/EEC. According to Fisk et al. (2003), TCPA appear as one of the substances for which the supply is expected to exceed or is exceeding more than 1,000 tonnes/year in the EU. Solutia, Inc. (2002) has reported that the substance is primarily used as an intermediate in the production of dyes and pigments but also used as a flame retardant in plastics. In this use the substance is present in the polymer matrix in reacted form. No information is available about the behaviour of hexachlorobenzene impurity in this use.

3 CLASSIFICATION AND LABELLING

Classification and labelling according to the 28th ATP of Directive 67/548/EEC:

Classification

Xn; R41	Risk of serious damage to eyes
Xn; R42/R43	May cause sensitisation by inhalation and skin contact
N; R50-53	Very toxic to aquatic organisms. May cause long-term adverse effects in the aquatic environment

The environmental classification was based on QSAR estimations.

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 508 days for the reaction with OH-radicals using AOP v1.91 (with TGD defaults: 24 h day^{-1}; $5*10^5$ OH^- cm^{-3}).

TCPA is an anhydride, a reactive species known to be hydrolysable (Smith and March, 2001). The presence of the electron-withdrawing chloro- groups of TCPA are expected to increase the susceptibility to base hydrolysis by reducing the electron density at the carbonyl carbon and making the meta carboxyl group a better leaving group. Thus, the tetrachloro- compound should hydrolyse even more rapidly than phthalic anhydride, which is reported to have a $T_{1/2}$ in water of about 90 seconds (Jones, 1972). TCPA can be expected to hydrolyse to its acid (US EPA, 1982).

A study submitted by industry (UCB, 2003) confirms the abovementioned hypothesis. In this study TCPA was tested in two ways to confirm that TCPA hydrolysis product is its acid form and to demonstrate under different isocratic conditions the hydrolysis of TCPA. HPLC with UV detector was used in the study for analysis.

In the first test the chromatograms confirm that the hydrolysis product of TCPA is its acid form. The formation of this product from TCPA was observed simultaneously with the disappearance of TCPA. The corresponding acid form is tetrachlorophthalic acid (CAS 632-58-6).

Under different isocratic elution conditions, increases of the water percentages of the eluent showed decreases of the TCPA elution peaks. This indicated that a hydrolytic reaction of TCPA takes place in the analysis system. When the amount of water was increased to 60%, TCPA peak disappeared. The highest TCPA retention time was 10 minutes, whereas the acid retention times were 2 minutes in all chromatograms.

Also the acid was tested under different isocratic conditions and the result was that the acid form is stable in water.

The conclusion of this study is that TCPA hydrolyses to its acid form in a matter of minutes and that the acid form is stable against further hydrolysis.

Other evidence of a rapid degradation provide Yu and Atallah (1978), who tested a structurally similar chemical tetrabromophthalic anhydride (TBPA, CAS 632-79-1). When TBPA was applied to silica gel surfaces and irradiated with UV light, it was demonstrated to hydrolyse rapidly (half life of less than 5 min.) to its dicarboxylic acid form; this result is also consistent with its degradation pattern in moist soil (Butz and Atallah, 1979). A similar, rapid hydrolysis after UV exposure could be expected to occur with TCPA.

4.1.2 Biotic degradation

Data not reviewed for this report.

4.1.3 Other information [1]

Data not reviewed for this report.

4.1.4 Summary and discussion of persistence

Based on the hydrolysis test of UCB (2003) and other supporting data from structurally similar substances, TCPA is considered to hydrolyse very fast in the presence of water. The hydrolysis product is based on the elution behavior its acid form tetrachlorophthalic acid (CAS 632-58-6). This substance is hydrolytically stable. Further assessment of the degradation of the hydrolysis product was not carried out.

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]

Tetrachlorophthalic anhydride has a calculated logKow of 4.65. The hydrolysis product tetrachlorophtalic acid (CAS 632-58-6) has an estimated logKow of 3.6 according to KOWWIN v1.67 .

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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 of tetrachlorophthalic anhydride or its hydrolysis product are available.

4.3.3 Other supporting information[4]

Data not reviewed for this report.

4.3.4 Summary and discussion of bioaccumulation

No experimental data on bioaccumulation of the parent compound or its hydrolysis product are available. Despite the high calculated logKow (4.65), it is considered that it is not necessary to assess further the bioaccumulation potential of tetrachlorophthalic anhydride. Due to the fast hydrolysis, exposure of the environment to the substance is unlikely or very low. The stable hydrolysis product tetrachlorophthalic acid has an estimated logKow of 3.6. It is concluded that the stable degradation product of the substance does not have high bioaccumulation potential.

5 HUMAN HEALTH HAZARD ASSESSMENT

Data not reviewed for this report.

6 ENVIRONMENTAL HAZARD ASSESSMENT

Data not reviewed for this report.

6.1 Aquatic compartment (including sediment)

6.1.1 Toxicity test results

6.1.1.1 Fish

Acute toxicity

Long-term toxicity

[3] For example, fish bioconcentration factor

[4] For example, measured concentrations in biota

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: tetrachlorophtalic anhydride (TCPA) does not meet the P criterion due to a fast hydrolysis. Based on a hydrolysis test and supporting evidence from structurally similar substances, TCPA is expected to hydrolyse to its acid form. The hydrolysis product is tetrachlorophthalic acid (CAS 632-58-6). This product is hydrolytically stable. Further degradation of the hydrolysis product was not assessed.

Bioaccumulation: TCPA meets the screening B criterion based on an estimated logKow of 4.65, but its bioaccumulation potential was not further assessed due to the fast hydrolysis. The hydrolysis product tetrachlorophthalic acid has an estimated logKow of 3.6 and it therefore does not meet the screening B criterion. No experimental data on bioaccumulation are available for TCPA or its hydrolysis product.

Toxicity: the available data were not reviewed for this report.

Other: commercially available tetrachlorophthalic anhydride may contain hexachlorobenzene (substance Nr. 59 of the PBT candidate list; CAS 118-74-1) as an impurity. The concentration of the impurity varies from < 0.1% w/w to 0.5% w/w depending on the producer/importer. Hexachlorobenzene is a persistent organic pollutant (POP) subject to Regulation 2004/850/EC.

Summary: pure tetrachlorophthalic anhydride does not meet the P criterion due to a fast hydrolysis. The substance meets the screening B criterion but its bioaccumulation potential was not assessed further due to the fast hydrolysis. The hydrolysis product tetrachlorophthalic acid (CAS 632-58-6) does not meet the screening B criterion. Ecotoxicity of tetrachlorophthalic anhydride or its acid was

not evaluated. It is concluded that tetrachlorophthalic anhydride as a pure substance is not considered as a PBT substance. Commercially available tetrachlorophthalic anhydride may contain hexachlorobenzene (CAS 118-74-1) as an impurity. Hexachlorobenzene is subject to Regulation 2004/850/EC.

INFORMATION ON USE AND EXPOSURE

Data not reviewed for this report.

OTHER INFORMATION

The information and references used in this report were taken from the following sources:

Butz RG and Atallah YH (1979) Effects of PHT-4 on soil microflora at level of 10 mg/g. Velsicol Chemical Corp. Chicago, Il. NTIS OTS0523290 (as cited in U.S.EPA, 2002).

Fisk PR, Girling AE and Wildey RJ (2003) Prioritisation of flame retardants for environmental risk assessment. Environment Agency (UK).

IPCS (1994) International Chemical Safety cards, nr. 1374.

Jones HR (1972) Environmental Control in the Organic and Petroleum Industries, Noyes Data Corp. New York, NY, USA, as cited in Dictionary of Substances and their Effects, 2nd Electronic Edition (as cited in U.S.EPA, 2002).

Smith MS and March J (2001) March's Advanced Organic Chemistry, 5th Ed. Wiley Interscience, pp 469.

Solutia Inc. (2002) IUCLID Dataset, tetrachlorophtalic anhydride , CAS 177-08-8, 02.11.2002. Submitted to the U.S.EPA HPV Chemicals Challenge Program.

Solutia, Inc. (2002b) High Production Volume (HPV) Chemicals Challenge Program. Test Plan for 4,5,6,7-tetrachloro-1,3-isobenzofurandione, CAS 117-08-8. Prepared by Solutia, Inc, received by U.S.EPA, November 8, 2002.

UCB (2003) Hydrolysis of Tetrachlorophthalic anhydride (Tetrathal). PASC Analytical Request #: 28789, NBP #: 1125172-73, Surface Specialties.

US EPA (1982) Preliminary Information Review-Tetrachlorophthalic Anhydride. PIR-317. EPA Contract No. 68-01-5789 (as cited in U.S.EPA, 2002).

Yu CC and Atallah YH (1978) Photolysis of PHT-4. Velsicol Chemical Corp. Ann Arbor, MI. NTIS OTS0523289 (as cited in U.S.EPA, 2002).