TC NES SUBGROUP ON IDENTIFICATION OF PBT AND VPVB SUBSTANCES

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

Substance name: 4-chloro-1-(2,4-dichlorophenoxy)-2-nitrobenzene

EC number: 219-244-6

CAS number: 2392-48-5

Molecular formula: C12H6Cl3NO3

Structural formula:

Summary of the evaluation:

4-chloro-1-(2,4-dichlorophenoxy)-2-nitrobenzene is not considered to be a PBT substance. It does not meet the B/vB criteria based on screening data. It may meet the P/vP criteria according to screening data. Assessment of ecotoxicity was not completed.

JUSTIFICATION

1 IDENTIFICATION OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

Name: 4-chloro-1-(2,4-dichlorophenoxy)-2-nitrobenzene

EC Number: 219-244-6 CAS Number: 2392-48-5

IUPAC Name:

Molecular Formula: C12H6Cl3NO3

Structural Formula:

Molecular Weight: 318.55

Synonyms: 2',4',4,2-dichloronitrodiphenyl ether; TNDE

1.1 Purity/Impurities/Additives

No data available.

1.2 Physico-Chemical properties

Table 1 Summary of physico-chemical properties. For references, see European Commission (2000)

REACH ref Annex, §	Property	Value	Comments
V, 5.1	Physical state at 20 C and 101.3 Kpa	solid	
V, 5.2	Melting / freezing point	80-82°C	Industrie Chimique Mulhouse Dornach (1995) (data not evaluated)
V, 5.3	Boiling point	224°C (at 8 hPa)	Industrie Chimique Mulhouse Dornach (1995) (data not evaluated)
V, 5.5	Vapour pressure	-	
V, 5.7	Water solubility	2.128 mg I-1 (at 25°C)	WSKOW v1.41
V, 5.8	Partition coefficient n- octanol/water (log value)	4.96 3.82	KOWWIN v1.67 Rhone-Poulenc (1996a)
VII, 5.19	Dissociation constant	-	

2 MANUFACTURE AND USES

One company has notified the substance under Regulation 93/793/EEC.

3 CLASSIFICATION AND LABELLING

The 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

No experimental data are available on abiotic degradation.

Indirect photochemical degradation in the atmosphere is considered to be very slow based on the estimated half-life of 22 days for the reaction with OH-radicals using AOP v1.91 (24 h day⁻¹; 5*10⁵ OH⁻ cm⁻³).

4.1.2 Biotic degradation

A test on ready biodegradability according to Directive 92/69/EEC, C.4-C (equivalent to OECD 301B) resulted by day 28 a degradation of < 1%. Domestic sludge and a test concentration corresponding to 40 mg organic carbon kg⁻¹ were used (Rhone Poulenc, 1997). The test is considered valid. BIOWIN v4.02 predictions support this finding.

4.1.3 Other information ¹

No data available.

4.1.4 Summary and discussion of persistence

No data are available on abiotic degradation. According to the available standard ready biodegradability test of Rhone Poulenc (1997) the substance is not readily biodegradable. In the lack of other experimental data, the substance is considered potentially persistent.

4.2 Environmental distribution

Data not reviewed for this report.

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

4.2.1 Adsorption

4.2.2 Volatilisation

4.2.3 Long-range environmental transport

4.3 Bioaccumulation (B)

4.3.1 Screening data2

A measured logKow of 3.82 and an estimated logKow of 4.96 are available for the substance. The experimental value is considered reliable (the test is valid). BCFWIN v2.14 provides a BCF of 174.3 using the first value.

4.3.2 Measured bioaccumulation data³

No experimental data on bioaccumulation are available for the substance.

4.3.3 Other supporting information⁴

No data available.

4.3.4 Summary and discussion of bioaccumulation

No experimental data on bioaccumulation are available. Based on the experimental logKow of 3.82, it can be expected that the substance has a moderate to high bioaccumulation potential. Testing would be necessary to determine the actual bioaccumulation potential.

5 HUMAN HEALTH HAZARD ASSESSMENT

Data not reviewed for this report.

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

³ For example, fish bioconcentration factor

⁴For example, measured concentrations in biota

6 ENVIRONMENTAL HAZARD ASSESSMENT

6.1 Aquatic compartment (including sediment)

6.1.1 Toxicity test results

6.1.1.1 Fish

Acute toxicity

No data available.

Long-term toxicity

No data available.

6.1.1.2 Aquatic invertebrates

Acute toxicity

For *Daphnia magna* an EC₅₀ (48 hours) of ca. 0.26 mg l^{-1} was determined by Rhone Poulenc, (1996b, 1996c) in a test according to Directive 92/69/EEC, C.2. The test concentration was measured in one of the test vessels at 0 hours (0.235 mg l^{-1}), at 24 hours (0.27 mg l^{-1}) and at 48 hours (0.26 mg l^{-1}). The test is considered to be valid.

Long-term toxicity

No data available.

6.1.1.3 Algae and aquatic plants

No data available.

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: 4-chloro-1-(2,4-dichlorophenoxy)-2-nitrobenzene may meet the P/vP criteria based on screening data. The substance was not readily biodegradable in a standard CO₂-evolution -test.

Bioaccumulation: the substance does not fulfil the B/vB criteria according to screening data. The available experimental logKow is 3.82, which is below the screening trigger of 4.5.

Toxicity: no long-term data are available on the effects of the substance to biota. Only one short-term test on its effects to *Daphnia magna* with an approximate EC_{50} (48 hours) of 0.26 mg I^{-1} was determined for the substance. It is not possible to evaluate the ecotoxicity on the basis of the available data. Long-term testing would be necessary to complete the assessment of ecotoxicity. However, such testing is not needed in the frame of this assessment due to the overall conclusion (see below).

Summary: 4-chloro-1-(2,4-dichlorophenoxy)-2-nitrobenzene does not meet the B/vB criteria based on screening data. It may meet the P/vP criteria according to screening data. Assessment of ecotoxicity was not completed. 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 taken from the following source:

European Commission (2000) IUCLID Dataset, 4-chloro-1-(2,4-dichlorophenoxy)-2-nitrobenzene, CAS 2392-48-5, 18.2.2000.

Other sources:

Rhone Poulenc (1996a) Determination du coefficient de partage n-octanol/eau du 2′,4′,2,4 trichloro-nitrodiphenylether ou TNDE. Selon les lignes directrices OCDE N° 107, CEEA8, ET NF 20-043. Etude n° 96/148 ENH/ENV

Rhone Poulenc (1996b) Determination de l'ecotoxicite aigue apres 24 heures et 48 heures de 2',4',2,4 trichloro-nitrodiphenylether (TNDE) vis avis de *Daphnia magna*. Selon la methode C.2 publiee dans le journal officiel des communautes europeennes le 19.12.92 (eesai en statique). Rapport l'etude D303.

Rhone Poulenc (1996c) Determination de l'ecotoxicite aigue apres 24 heures et 48 heures de 2′,4′,2,4 trichloro-nitrodiphenylether (TNDE) vis avis de *Daphnia magna*. Dosage du TNDE. Etude n° 96/160

Rhone Poulenc (1997) Evaluation en milieuaqueux de la biodegradabilite aerobie "ultime" de 2′,4′,2,4 trichloro-nitrodiphenylether (TNDE). Selon la methode publiee dans le journal officiel des communautes europeennes du 29 decembre 1992 (mothode C4-C par analyse du dioxyde de carbone degage). Rapport del'etude BD121.