

TC NES SUBGROUP ON IDENTIFICATION OF PBT AND VPVB SUBSTANCES

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

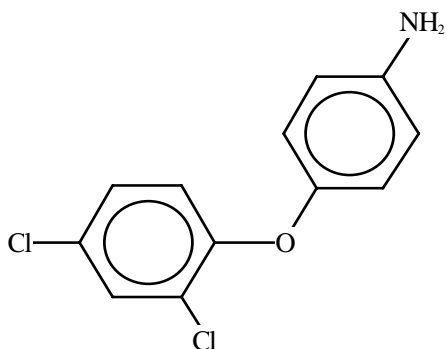
Substance name: 4-(2,4-dichlorophenoxy)aniline

EC number: 238-932-7

CAS number: 14861-17-7

Molecular formula: C₁₂H₉Cl₂NO

Structural formula:



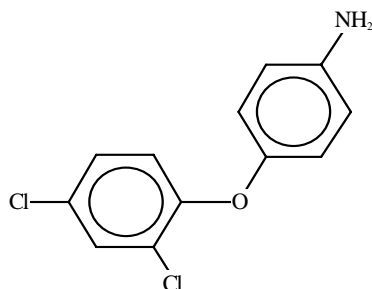
Summary of the evaluation:

The substance is not considered to be a PBT substance. It does not meet the B criterion based on screening data. It may meet the P/vP criteria according to screening data. The assessment of ecotoxicity was not completed.

JUSTIFICATION

1 IDENTIFICATION OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

Name: 4-(2,4-dichlorophenoxy)aniline
EC Number: 238-932-7
CAS Number: 14861-17-7
IUPAC Name:
Molecular Formula: C₁₂H₉Cl₂NO
Structural Formula:



Molecular Weight: 254.12
Synonyms: Aminofen; 2,4-dichloro-1-4(aminophenoxy)benzene; 2,4-dichloro-4'-amonodiphenylether; for the complete 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 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	61-63°C	Hoechst AG (1994) (data not evaluated)
V, 5.3	Boiling point	180°C (at 4 hPa)	Hoechst AG (1994) (data not evaluated)
V, 5.5	Vapour pressure	0.000004 hPa (at 20°C) < 0.1 hPa (at 20°C)	Hoechst AG (1992) (data not evaluated) Hoechst AG (1994) (data not evaluated)
V, 5.7	Water solubility	16.5 mg l ⁻¹ (at 20°C) 17.1 mg l ⁻¹ (at 20°C) 19.6 mg l ⁻¹ (at 25°C)	Hoechst AG (1992) (data not evaluated) Hoechst AG (1992) (data not evaluated) Calculated (WSKOW v1.41)
V, 5.8	Partition coefficient n-octanol/water (log value)	3.58 4.6 (at 25°C) 3.8 (at 20°C)	Calculated (KOWWIN v1.67) Calculated (CLOGP3; Hoechst AG, 1992) AllessaChemie GmbH (2003); HPLC-method (92/69/EC, A.8)
VII, 5.19	Dissociation constant	-	

2 MANUFACTURE AND USES

Two companies have provided information on the substance under Regulation 93/793/EEC. According to industry, one producer and one user operate presently in Europe.

3 CLASSIFICATION AND LABELLING

The substance is not classified in the Annex I of Directive 67/548/EEC. The producer has classified the substance provisionally with T; R45 (may cause cancer), T; R20/21/22 (harmful by inhalation, in contact with skin and if swallowed), N; R50/53 (very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment).

4 ENVIRONMENTAL FATE PROPERTIES

4.1 DEGRADATION (P)

4.1.1 Abiotic degradation

One study on photodegradation of 4-(2,4-dichlorophenoxy)aniline (aminofen) has been reported by Draper and Casida (1983). In this study aminofen was exposed as a thin film (90 µg cm⁻²) to 360 nm light. The author reported a half-life of one hour for phototransformation and that as a main product nitrofen was identified. However, the study lacks all relevant details and the results are therefore not considered as reliable. Environmentally relevant exposure occurs in the whole water column and, in the case of this substance, especially in sediment and soil. Photodegradation of the

substance can be expected to be a relevant removal pathway in the environment only in very shallow clear waters and in the first few centimetres layer of the water column. Aquatic photodegradation is not considered to have relevant impact on the overall persistency of the substance in the environment.

The substance is not expected to hydrolyse under environmentally relevant conditions.

Indirect photochemical degradation in the atmosphere is considered to be fast based on the estimated half-life of 5.4 hours for the reaction with OH-radicals using AOP v1.91 (24 h day⁻¹; $5 \cdot 10^5 \text{ OH}^- \text{ cm}^{-3}$).

4.1.2 Biotic degradation

A test on ready biodegradability according to OECD 301D (closed bottle test) resulted in 28 days an oxygen consumption of < 20% measured as % of ThOD. Domestic sludge and a test concentration of 13 mg l⁻¹ were used. It is noted that the study report was not available to the Rapporteur for evaluation. BIOWIN v4.02 predictions support the result.

4.1.3 Other information ¹

No data available.

4.1.4 Summary and discussion of persistence

Aminofen is not readily biodegradable according to the available standard OECD 301D –test. The low degree of degradation reached within 28 days indicates that the substance may be persistent. Abiotic degradation is not expected to be relevant for this type of substance.

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

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

4.3 BIOACCUMULATION (B)

4.3.1 Screening data²

An experimental logK_{ow} of 3.8 was derived using the HPLC method according to Directive 92/69/EC A.8 by AllessaChemie (2003). This result is considered reliable. A BCF of 168.3 was derived by BCFWIN v2.15 using this 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

Based on the experimental logK_{ow} of 3.8, it is concluded that aminofen has a moderate to high bioaccumulation potential.

5 HUMAN HEALTH HAZARD ASSESSMENT

Data not reviewed for this report.

6 ENVIRONMENTAL HAZARD ASSESSMENT

6.1 AQUATIC COMPARTMENT (INCLUDING SEDIMENT)

6.1.1 Toxicity test results

6.1.1.1 Fish

Acute toxicity

A LC₅₀ (96 hours) of 0.5 mg l⁻¹ was obtained according to an APHA method from 1965 for *Lebistes reticulatus* (Hoechst AG, 1975) at 21-22°C. For *Salmo salar* a LC₅₀ (96 hours) of 0.51 mg l⁻¹ at 16°C was determined also by Hoechst AG (1975) using the same method. It is noted that the test reports were not available for the Rapporteur for evaluation.

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

³ For example, fish bioconcentration factor

⁴ For example, measured concentrations in biota

Long-term toxicity

No data available.

6.1.1.2 Aquatic invertebratesAcute toxicity

For the arthropod *Aedes aegypti* a LC₅₀ (96 hours) of 3.6 mg l⁻¹ (Hoechst AG, 1975) and for the mollusc *Planorbis corneus* a LC₅₀ (96 hours) of 4.2 mg l⁻¹ (Hoechst AG, 1975) have been determined (no standard tests). It is noted that the test reports were not available for the Rapporteur for evaluation.

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

Data available for effects on microorganisms were not reviewed for this report.

6.2 TERRESTRIAL COMPARTMENT

Data available for effects on plants were not reviewed for this report.

6.3 ATMOSPHERIC COMPARTMENT

No data available.

7 PBT AND VPVB**7.1 PBT, VPVB ASSESSMENT**

Persistence: 4-(2,4-dichlorophenoxy)aniline (aminofen) may meet the P/vP criteria based on screening data. The substance is not readily biodegradable according to a standard ready biodegradability test (OECD 301D). Further testing would be needed to examine the rate of biotic degradation. However, further testing is not required in the frame of this assessment due to the overall conclusion (see below).

Bioaccumulation: Aminofen does not meet the B criterion according to screening data. The available reliable experimental logK_{ow} is 3.8, which is below the screening trigger of 4.5.

Toxicity: No long-term data are available on the effects of aminofen to aquatic biota. The very few short term aquatic data indicate that the substance may not meet the T criterion. Long-term testing would be necessary to complete the assessment of ecotoxicity. However, such testing is not needed due to the overall conclusion (see below).

Summary: 4-(2,4-dichlorophenoxy)aniline does not meet the B criterion based on screening data. It may meet the P/vP criterion according to screening data. The 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-(2,4-dichlorophenoxy)aniline, CAS 14861-17-7, 18.2.2000.

Other sources:

AllessaChemie GmbH (2003) Determination of the Partition Coefficient [1-Octanol/Water] of Aminofen in accordance with EEC-Guideline A.8. Report No. B 018/2003. Report for Clariant GmbH, 04, June, 2003.