

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

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

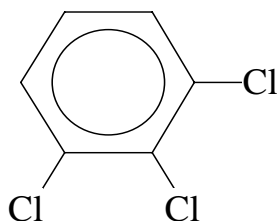
**Substance name:** 1,2,3-trichlorobenzene

**EC number:**

**CAS number:** 87-61-6

**Molecular formula:**

**Structural formula:**



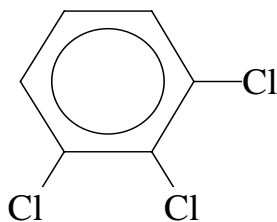
#### Summary of the evaluation:

Based on available information including QSAR –predictions, 1,2,3-trichlorobenzene (1,2,3-TCB) has very similar physical-chemical properties as 1,2,4-trichlorobenzene (1,2,4-TCB; see PBT summary fact sheet no. 4). Reading across from 1,2,4-TCB, P-criterion and B-criterion are considered fulfilled for 1,2,3-TCB. This conclusion is also supported by limited test data on 1,2,3-TCB. There are no long-term ecotoxicity test data available for 1,2,3-TCB, but based on structural similarity to 1,2,4-TCB, 1,2,3-TCB is expected to exhibit similar toxicity. Measured and modelled QSAR data on volatility, hydrophobicity, atmospheric degradation and water solubility indicate together with reading across from the properties of 1,2,4-TCB that 1,2,3-TCB is expected to have a similar high potential for long-range atmospheric transport. Therefore, overall 1,2,3-TCB is concluded to fulfil the PBT- criteria.

## JUSTIFICATION

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

Name: 1,2,3-trichlorobenzene  
EC Number: 201-757-1  
CAS Number: 87-61-6  
IUPAC Name: 1,2,3-trichlorobenzene  
Molecular Formula: C<sub>6</sub>H<sub>3</sub>Cl<sub>3</sub>  
Structural Formula:



Molecular Weight: 181.46  
Synonyms: 1,2,3-TCB (abbreviation)

#### 1.1 PURITY/IMPURITIES/ADDITIVES

#### 1.2 PHYSICO-CHEMICAL PROPERTIES

Table 1 presents some of the available data of unknown quality on the physical-chemical properties. The available data for 1,2,3-TCB are similar to the values available for 1,2,4-TCB. Furthermore, based on the close structural similarity with 1,2,4-TCB, it is not expected that 1,2,3-TCB would have physical-chemical properties significantly different from 1,2,4-TCB.

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	Liquid	
V, 5.2	Melting / freezing point		
V, 5.3	Boiling point	218 °C at 1,013 hPa	Bayer AG (data not evaluated)
V, 5.5	Vapour pressure	9.3 Pa at 20°C (reported as 0.093 mbar)	Bayer AG (data not evaluated)
V, 5.7	Water solubility	16 mg l <sup>-1</sup> at 25°C 18.8 mg l <sup>-1</sup> at 25°C 18 mg l <sup>-1</sup> 12 mg l <sup>-1</sup>	Bayer AG (data not evaluated) Calculated (WSKOW v1.41) Chicou et al. (1986) (exper. database of WSKOW v1.41; data not evaluated) Verschuieren (1983)(data not evaluated)
V, 5.8	Partition coefficient n-octanol/water (log value)	4.05 3.93	Sangster (1994)(exper. database of KOWWIN v1.67; data not evaluated) Calculated (KOWWIN v1.67)
VII, 5.19	Dissociation constant	-	

## 2 MANUFACTURE AND USES

According to industry, 1,2,3-trichlorobenzene (1,2,3-TCB) is planned to be produced in a volume of 1000 tpa in a closed system and to be sold to a limited number of customers, which would use it as intermediate. Note: this substance is registered as a LPVC and is produced at two sites according to ESIS.

## 3 CLASSIFICATION AND LABELLING

1,2,3-TCB 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

Indirect photochemical degradation in the atmosphere is considered to be very slow based on the estimated half-life of 57 days for the reaction with OH-radicals using AOP v1.91 (24 h day<sup>-1</sup>;  $5 \cdot 10^5 \text{ OH}^- \text{ cm}^{-3}$ ).

#### 4.1.2 Biotic degradation

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

#### 4.1.4 Summary and discussion of persistence

Both the abiotic and biotic degradability is expected to be similar to the close structural analog 1,2,4,-TCB. The biotic degradability could based on structural considerations and some evidence from literature be somewhat lower for 1,2,3-TCB than for 1,2,4-TCB (e.g. Marinucci and Bartha, 1979). In conclusion, 1,2,3- TCB is regarded to fulfil the P but not the vP criterion.

### 4.2 ENVIRONMENTAL DISTRIBUTION

#### 4.2.1 Adsorption

#### 4.2.2 Volatilisation

1,2,3-TCB can be classified generally as a volatile substance based on the vapour pressure of 9.3 Pa at 20°C. Henry's Law constant of 126 Pa m<sup>3</sup> mol<sup>-1</sup> was obtained using the mentioned vapour pressure (converted to 13.1 Pa at 25°C), the water solubility of 18.8 mg l<sup>-1</sup> at 25°C from Table 1 and the mole weight of 181.46 g mol<sup>-1</sup>. This value indicates very high volatility from water.

#### 4.2.3 Long-range environmental transport

As the physical-chemical properties of 1,2,3-TCB do not differ significantly from the properties of 1,2,4-TCB, atmosphere is assumed to be the main distribution route of 1,2,3-TCB. Based on the structural similarities and the available data, 1,2,3-TCB is also expected to have a very high potential for long-range atmospheric transport.

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

### **4.3 BIOACCUMULATION (B)**

#### **4.3.1 Screening data<sup>2</sup>**

#### **4.3.2 Measured bioaccumulation data<sup>3</sup>**

#### **4.3.3 Other supporting information<sup>4</sup>**

#### **4.3.4 Summary and discussion of bioaccumulation**

A BFC of 1,900 has been measured for fish (Van Hoogen and Opperhuizen, 1988). The data quality is unknown but may be reliable because this value is very similar to the BCF level of 1,2,4-TCB. Therefore, based on the structural similarity, 1,2,3-TCB is regarded as having similar bioaccumulation potential as 1,2,4-TCB, i.e., just fulfilling the B criterion but not the vB criterion.

## **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

##### Long-term toxicity

No test data on long-term fish toxicity are available.

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<sup>2</sup> For example, log  $K_{ow}$  values, predicted BCFs

<sup>3</sup> For example, fish bioconcentration factor

<sup>4</sup> For example, measured concentrations in biota

### **6.1.1.2 Aquatic invertebrates**

#### Acute toxicity

#### Long-term toxicity

No test data on long-term toxicity to aquatic invertebrates are available.

### **6.1.1.3 Algae and aquatic plants**

### **6.1.2 Sediment organisms**

No test data on toxicity to sediment organisms are available.

### **6.1.3 Other aquatic organisms**

No test data on toxicity to other aquatic organisms are available.

## **6.2 TERRESTRIAL COMPARTMENT**

Data not reviewed for this report.

## **6.3 ATMOSPHERIC COMPARTMENT**

Data not reviewed for this report.

# **7 PBT AND VPVB**

## **7.1 PBT, VPVB ASSESSMENT**

Based on available information including QSAR –predictions, 1,2,3-trichlorobenzene (1,2,3-TCB) has very similar physical-chemical properties as the structurally similar substance 1,2,4-trichlorobenzene (1,2,4-TCB; see PBT summary fact sheet no. 4). Based on limited evidence from experimental data on 1,2,3-TCB but supported by reading across from 1,2,4-TCB, the P-criterion and B-criterion are considered fulfilled also for 1,2,3-TCB. No long-term ecotoxicity data are available for 1,2,3-TCB, but based on the structural similarity with 1,2,4-TCB, 1,2,3-TCB is expected to have similar chronic toxicity to aquatic organisms. Therefore, the T criterion is probably not quite fulfilled for 1,2,3-TCB. Measured data and QSAR -model results available on volatility, hydrophobicity, atmospheric degradation and water solubility indicate together with reading across from properties of 1,2,4-TCB that 1,2,3-TCB is expected to have a similar high potential for long-range atmospheric transport as 1,2,4-TCB. Therefore, overall, 1,2,3-TCB is concluded to fulfil the PBT criteria.

## INFORMATION ON USE AND EXPOSURE

### OTHER INFORMATION

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

Bayer AG, Material Safety Data Sheet of Bayer Chemicals.

Marinucci AC and Bartha R (1979) *Appl. Env. Microbiology*, 38 (5), 811-17.

Van Hoogen G and Opperhuizen A (1988) *Env. Toxicol. Chem.*, 7(3), 213-219.

Verschueren (1983) *Handbook of Environmental data on Organic Chemicals* (2<sup>nd</sup> Ed. 1983)