

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

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

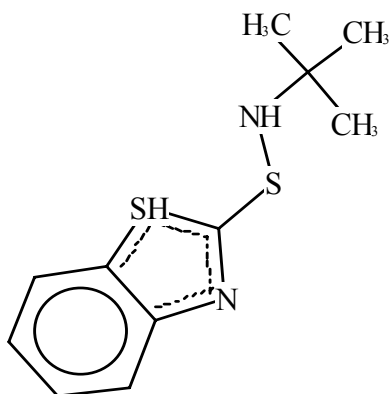
**Substance name:** N-tert-butylbenzothiazole-2-sulphenamide

**EC number:** 202-409-1

**CAS number:** 95-31-8

**Molecular formula:** C<sub>11</sub>H<sub>14</sub>N<sub>2</sub>S<sub>2</sub>

**Structural formula:**



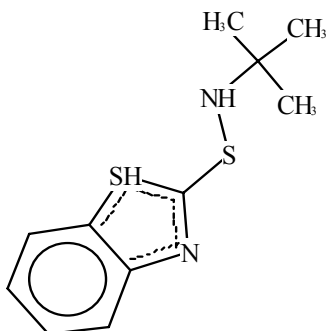
#### Summary of the evaluation:

N-tert-butylbenzothiazole-2-sulphenamide (TBBS) is not considered to be a PBT substance. It does not meet the P criterion due to a fast hydrolysis. Degradation of its identified hydrolysis products was not assessed for this report. TBBS is not likely to be subject to relevant bioaccumulation in the environment due to its fast hydrolysis. The hydrolysis products do not meet the B criterion. Ecotoxicity data were not reviewed for this report.

## JUSTIFICATION

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

Name: N-tert-butylbenzothiazole-2-sulphenamide  
EC Number: 202-409-1  
CAS Number: 95-31-8  
IUPAC Name:  
Molecular Formula: C<sub>11</sub>H<sub>14</sub>N<sub>2</sub>S<sub>2</sub>  
Structural Formula:



Molecular Weight: 238.37  
Synonyms: 2-benzothiazolesulphenamide, N-(1,1-dimethylethyl)-; N-1,1-(dimethylethyl)-2-benzothiazolesulphenamide; TBBS (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 references, see European Commission (2000) and OECD (2003)

REACH ref Annex, §	Property	Value	Comments
V, 5.1	Physical state at 20°C and 101.3 kPa	solid	European Commission (2000)
V, 5.2	Melting / freezing point	105°C	OECD (2003)
V, 5.3	Boiling point	unmeasurable (degrades at 207°C)	OECD (2003)
V, 5.5	Vapour pressure	< 0.0000021 (at 25°C)	OECD (2003)
V, 5.7	Water solubility	0.345 mg l <sup>-1</sup> (at 20°C) 177.7 mg l <sup>-1</sup> (at 25°C)	OECD (2003) WSKOW v1.41
V, 5.8	Partition coefficient n-octanol/water (log value)	3.9 (at room temperature) 4.38 4.67 (at 22.4°C) 2.56	OECD (2003) Monsanto (1992) (data not evaluated) Bayer AG data (data not evaluated) KOWWIN v1.67
VII, 5.19	Dissociation constant	pKa <sub>(1)</sub> 1.75, pKa <sub>(2)</sub> -3.43 (prediction); the substance is not ionised in environmentally relevant pH range	OECD (2003)

## 2 MANUFACTURE AND USES

Six companies have supplied information on the substance under Regulation 93/793/EEC. A quantity of 10,000-50,000 tonnes/annum is produced and/or imported in Europe. The substance is used, i.a., as a curing agent in rubber industry and as an intermediate (European Commission, 2000). According to Bayer (2003), the substance is solely used as a curing agent (accelerator) for the production of rubber.

## 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

According to OECD (2003), N-tert-butylbenzothiazole-2-sulphenamide (TBBS) is hydrolysed rapidly at pH ≤ 9 in water. METI (1996) conducted a test according to OECD 111. Hydrolysis half-lives of 1.7, 1.8 and 21.5 hours for pH 4, 7, and 9 were determined, respectively.

At 50 °C more than 50 % of the substance was hydrolysed in 2.4 hours at all pH values covered (4, 7, and 9) in a test according to OECD 111 (Bayer, 1997).

TBBS is expected to react in the hydrolysis in a similar way as in the curing process, where thermal decomposition of the substance occurs. During vulcanization the unstable sulphur-nitrogen bond of benzothiazole sulphenamides is split with an intermediate formation of a 2-mercaptobenzothiazole (CAS 149-30-4) radical. Products resulting from the decomposition process are basic amines, benzothiazole derivatives and further reaction products (GDCh, 1991). Primary hydrolysis products of TBBS are mercaptobenzothiazole (CAS 149-30-4) and t-butylamine (CAS 75-64-9) (Monsanto, 1984a and b) which are followed in the reaction chain by di(benzothiazoyl-2)disulphide (CAS 128-78-5) and benzothiazole (CAS 95-16-9) (for an overview of the degradation products, see e.g. European Commission, 2007).

Degradation properties of the hydrolysis products were not reviewed for this report.

Indirect photochemical degradation in the atmosphere is considered to be fast for TBBS based on the estimated half-life of 8.4 hours for the reaction with OH-radicals using AOP v1.91 (24-h day<sup>-1</sup>;  $5 \cdot 10^5$  [OH] cm<sup>-3</sup>).

#### 4.1.2 Biotic degradation

Based on a ready biodegradability test (OECD 301 C), 0% of the substance was degraded in 28 days (Bayer AG data as cited in European Commission, 2000). It is noted that the study report was not available to the Rapporteur for evaluation. Due to the fast hydrolysis of the substance, the test has probably measured biodegradation of hydrolysis products.

Another screening biodegradability test according to Monsanto shake flask procedure (test concentration 29.4 mg l<sup>-1</sup>) using adapted inoculum resulted in a biodegradation of 63.5% (ThCO<sub>2</sub>) in 32 days (European Commission, 2000). The result cannot be used for screening biodegradation assessment without other supporting evidence due to the adapted inoculum and a low test concentration. It is noted that the study report was not available to the Rapporteur for evaluation.

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

Data not reviewed for this report.

#### 4.1.4 Summary and discussion of persistence

TBBS undergoes a rapid hydrolysis according to the available OECD 111 test results and the substance is hence considered as not persistent. Data on the degradation of the hydrolysis products were not further reviewed for this report since they are not considered as PBT substances due to their low bioaccumulation potential.

Based on the available ready biodegradability test according to OECD 301C, the substance is considered as not readily biodegradable. However, due to the fast hydrolysis, it is noted, that the test result has probably measured biodegradation of the hydrolysis products.

## 4.2 ENVIRONMENTAL DISTRIBUTION

Data not reviewed for this report.

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<sup>1</sup> 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 data<sup>2</sup>**

The available logK<sub>ow</sub> values are between 2.56 and 4.67. A BCF of 787 was derived by BCFWIN v2.15 (logK<sub>ow</sub> of 4.67 used).

For degradation products mercaptobenzothiazole, di(benzothiazoyl-2)disulphide and benzothiazole logK<sub>ow</sub> –values from approximately 2 to 4.5 are available (see European Commission, 2007; OECD, 2003). For t-butylamine, a logK<sub>ow</sub> of 0.72 was estimated by KOWWIN v1.67.

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

No experimental data on bioaccumulation are available for TBBS.

BCFs of < 8 -51 have been derived experimentally for fish for the hydrolysis products mercaptobenzothiazole, di(benzothiazoyl-2)disulphide and benzothiazole (for details, see European Commission, 2007 and OECD, 2003).

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

Data not reviewed for this report.

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

No experimental data on bioaccumulation are available for TBBS. Due to the fast hydrolysis, significant bioaccumulation is not expected to occur in the environment. Further bioaccumulation testing of TBBS is not considered necessary for this assessment. The hydrolysis products have a low bioaccumulation potential based on their logK<sub>ow</sub>-values and/or experimental bioaccumulation data.

## **5 HUMAN HEALTH HAZARD ASSESSMENT**

Data not reviewed for this report.

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<sup>2</sup> For example, log K<sub>ow</sub> values, predicted BCFs

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

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

## **6 ENVIRONMENTAL HAZARD ASSESSMENT**

### **6.1 AQUATIC COMPARTMENT (INCLUDING SEDIMENT)**

Data not reviewed for this report.

#### **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: N-tert-butylbenzothiazole-2-sulphenamide (TBBS) does not meet the P criterion due to a rapid hydrolysis observed in two OECD 111 -tests. Degradation of the identified hydrolysis products was not further reviewed for this report since they are not considered as PBT substances due to their low bioaccumulation potential.

Bioaccumulation: No experimental data on bioaccumulation of TBBS are available. However, the substance is not likely to be subject to relevant bioaccumulation due to its fast hydrolysis. The identified hydrolysis products do not meet the B criterion based on the available logKow –values and/or experimental BCF-values.

Toxicity: Data on ecotoxicity were not reviewed for this report.

Summary: N-tert-butylbenzothiazole-2-sulphenamide (TBBS) does not meet the P criterion due to a fast hydrolysis. Degradation of its identified hydrolysis products was not assessed for this report. TBBS is not likely to be subject to relevant bioaccumulation in the environment due to its fast hydrolysis. The hydrolysis products do not meet the B criterion. Ecotoxicity data were not reviewed for this report. 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 two main sources:

European Commission (2000) IUCLID Dataset, N-tert-butylbenzothiazole-2-sulphenamide, CAS 95-31-8, 19.2.2000.

OECD (2003) SIDS Initial Assessment Report for SIAM 16, Paris, France, 27-30 May, 2003, N-tert-butylbenzothiazole-2-sulphenamide, CAS 95-31-8. UNEP Publications.

Other sources:

Bayer (1997) Abiotic degradation of N,N-Dicyclohexylbenzothiazole-2-sulphenamid and N-tert-Butyl-2-benzothiazolesulphenamid as a function of pH according to the OECD test guideline 111. Antwerpen, 20.05.1997.

Bayer (2003) Personal communication. Email by Dr. Burkhardt Stock (Bayer) to German Federal Environment Agency on 24<sup>th</sup> April 2003.

European Commission (2007) European Risk Assessment Report, Draft of 04.07.2007, N-cyclohexylbenzothiazole-2-sulphenamide, CAS No: 95-33-0, EINECS No: 202-411-2.

METI (1996) Ministry of Economy, Trade and Industry (formerly MITI), Japan, unpublished data, conducted by Chemicals Evaluation and Research Institute (CERI, Japan), Test No: 21219K.

Mosanto (1984a) Monsanto Study AB-84-X128.

Monsanto (1984b) Monsanto Study AB-84-X133.