

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

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

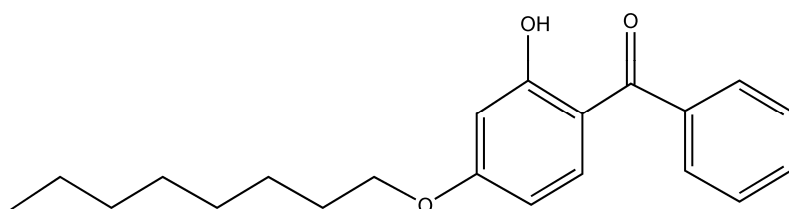
**Substance name:** Octabenzone

**EC number:** 217-421-2

**CAS number:** 1843-05-6

**Molecular formula:** C<sub>21</sub>H<sub>26</sub>O<sub>3</sub>

**Structural formula:**



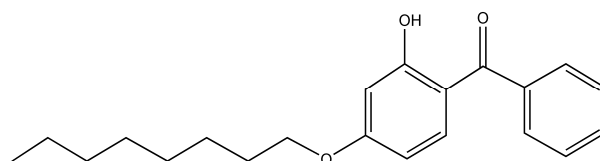
#### Summary of the evaluation:

Octabenzone is not considered to be a PBT substance. It does not meet the B criterion. The screening P/vP criteria are fulfilled.

## JUSTIFICATION

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

Name: Octabenzene  
 EC Number: 217-421-2  
 CAS Number: 1843-05-6  
 IUPAC Name:  
 Molecular Formula: C<sub>21</sub>H<sub>26</sub>O<sub>3</sub>  
 Structural Formula:



Molecular Weight: 326.4  
 Synonyms: 2-hydroxy-4-n-octoxy-benzophenon

#### 1.1 PURITY/IMPURITIES/ADDITIVES

No data available.

#### 1.2 PHYSICO-CHEMICAL PROPERTIES

Table 1 Summary of physico-chemical properties. For details and 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	48-49°C	Ciba-Geigy (data not evaluated)
V, 5.3	Boiling point		
V, 5.5	Vapour pressure		
V, 5.7	Water solubility	< 1 mg l <sup>-1</sup> (at 20°C) 0.037 mg l <sup>-1</sup> (at 25°C)	Ciba-Geigy (data not evaluated) Calculated (WSKOW v1.41)
V, 5.8	Partition coefficient n-octanol/ water (log value)	> 6 6.96	Ciba-Geigy (data not evaluated) Calculated (KOWWIN v1.67)
VII, 5.19	Dissociation constant		

## 2 MANUFACTURE AND USES

Five companies have provided information on the substance under Regulation 93/793/EEC. The substance has according to European Commission (2000) such applications as use as an additive and antioxidant. The industrial category which has been specified is polymer industry.

## 3 CLASSIFICATION AND LABELLING

The substance is not classified according to 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 fast based on the estimated half-life of 1.8 hours for the reaction with OH-radicals using AOP v1.91 (24 h day<sup>-1</sup>;  $5 \cdot 10^5$  OH<sup>-</sup> cm<sup>-3</sup>).

#### 4.1.2 Biotic degradation

Ciba-Geigy SpA has reported on a test according to OECD 301 B. A use of anaerobic bacteria is mentioned, although the test standard measures degradation in aerobic conditions. Test concentration was 20.1 mg l<sup>-1</sup> and test duration 28 days. 5% degradation was observed at the end of the test measured as CO<sub>2</sub> –evolution. According to the result, the substance is considered to be not readily biodegradable. It is noted that the test report was not available to the Rapporteur for evaluation.

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

#### 4.1.4 Summary and discussion of persistence

Based on the available test according to OECD 301 B, the substance is considered not readily biodegradable.

## 4.2 ENVIRONMENTAL DISTRIBUTION

Data not reviewed for this report.

### 4.2.1 Adsorption

### 4.2.2 Volatilisation

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

### 4.2.3 Long-range environmental transport

## 4.3 BIOACCUMULATION (B)

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

A BCF of 209.5 was predicted by BCFWIN v2.15 using the calculated logK<sub>ow</sub> of 6.96.

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

CERI (2003) has reported on a test who measured bioconcentration in *Cyprinus carpio* in a flow-through system according to OECD 305. Test duration was 60 days, DMF was used as dispersant in concentration of 19 mg l<sup>-1</sup> and test concentrations were 0.2 and 2 µg l<sup>-1</sup>. BCFs were reported as the relation of the measured concentration in water (measured with HPLC) and fish (measured with LC/MS-MS). The results are presented below.

#### Measured concentration in test water

Level/Duration	14 days	28 days	42 days	53 days	60 days
2 µg l <sup>-1</sup>	2.06	2.08	2.12	1.94	2.01
0.2 µg l <sup>-1</sup>	0.185	0.187	0.206	0.203	0.188

#### BCF value:

Level/Duration	14 days	28 days	42 days	53 days	60 days
2 µg l <sup>-1</sup>	110	170	89	190	180
	130	100	150	190	160
0.2 µg l <sup>-1</sup>	100	150	100	140	120
	120	150	70	72	94

Based on the measured concentrations it is considered that steady state was reached during the test. The lower test concentration was below water solubility although dispersant was used. The results are considered reliable enough for the purpose of this assessment. It is concluded that measured BCF for fish is below 200.

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

Data not available.

<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

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

The predicted BCF of 209.5 is in the same range as the BCF (< 200) derived experimentally according to OECD 305. It can be concluded that the substance has a low to moderate 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

###### **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:** Octabenzene meets the screening P/vP criteria. It is considered not readily biodegradable based on a test according to OECD 301 B.

**Bioaccumulation:** The substance does not meet the B criterion. An experimental BCF determined according to OECD 305 was observed to be below 200.

**Toxicity:** Data available were not reviewed for this report.

**Summary:** Octabenzene does not meet the B criterion. It is considered to meet the screening P/vP criteria. Assessment of ecotoxicity was not conducted. It is concluded that octabenzene 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 mainly taken from the following source:

European Commission (2000) IUCLID Dataset, octabenzene, CAS 1843-05-6, 18.2.2000.

Other sources:

CERI (2003) Information provided on CERI bioconcentration tests to the ECB.