

THIS DOCUMENT HAS BEEN PREPARED ACCORDING TO THE PROVISIONS OF ARTICLE 136(3) “TRANSITIONAL MEASURES REGARDING EXISTING SUBSTANCES” OF REACH (REGULATION (EC) 1907/2006). IT IS NOT A PROPOSAL FOR A RESTRICTION ALTHOUGH THE FORMAT IS THE SAME

**Annex XV dossier**

**Transitional Dossier**

**CAS No.**            **100-41-4**

**EINECS No.**        **202-849-4**

**IUPAC Name**        **Ethylbenzene**

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## TABLES

Table 1: Summary of physico- chemical properties

.....**Erro**  
**r! Bookmark not defined.**

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## **RESTRICTION PROPOSAL**

CAS No. 100-41-4

EINECS No. 202-849-4

IUPAC Name Ethylbenzene

**Restriction proposal:** None

Other Risk reduction measures see attached Risk Reduction Strategy.

## INFORMATION ON HAZARD AND RISKS

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

#### 1.1 Name and other identifiers of the substance

CAS No. 100-41-4

EINECS No. 202-849-4

IUPAC Name Ethylbenzene

#### 1.2 Composition of the substance

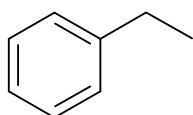
CAS Number: 100-41-4

EINECS Number: 202-849-4

IUPAC Name: Ethylbenzene

Molecular formula:  $C_8 H_{10}$

Structural formula:



Molecular weight: 106 g/mol

Synonyms: Ethylbenzol

Benzene, ethyl-  
alpha.-Methyltoluene

### 1.3 Physico-chemical properties

#### **Vapour Pressure**

The vapour pressure of a substance is defined as the saturation pressure above a solid or liquid substance. At the thermodynamic equilibrium, the vapour pressure of a pure substance is a function of the temperature only.

Vapour pressures in the range of 1 mm mercury column (1.333 hPa) at  $-9.8\text{ }^{\circ}\text{C}$  to 760 mm (1013.25 hPa) mercury column at  $136.2\text{ }^{\circ}\text{C}$  are listed in the CRC Handbook of Chemistry and Physics (Lide, 1991-1992)

A value of 9.3 hPa at  $20\text{ }^{\circ}\text{C}$  is listed in the Auer Technikum (1988) which is a collection of common tables of several chemical compounds and is often used in laboratories. This value has been used for further calculations. 16 hPa at  $30\text{ }^{\circ}\text{C}$  and 46 hPa at  $50\text{ }^{\circ}\text{C}$  are also mentioned in the Auer Technikum. These values are also in good agreement with the values mentioned in the CRC Handbook.

A value of 9.33 hPa at  $20\text{ }^{\circ}\text{C}$  is mentioned by Verschueren (1983) and Duve et al. (1976) which supports the value of the Auer Technikum (1988).

Moreover Verschueren (1983) mentions a value of 16 hPa at  $30\text{ }^{\circ}\text{C}$ . This value is in good agreement with the Auer Technikum and the CRC Handbook.

#### **Water Solubility**

The water solubility of a substance is specified by its saturation concentration in pure water at a certain temperature, preferably at  $20\text{ }^{\circ}\text{C}$ .

A water solubility of 160 mg/l at  $25\text{ }^{\circ}\text{C}$  is mentioned in the CRC Handbook of Chemistry and Physics (Lide, 1991-1992). This value is in very good agreement with other values and has been used for further calculations therefore.

A value of 152 mg/l at  $20\text{ }^{\circ}\text{C}$  is mentioned by Tewari et al. (1982) and Verschueren (1983) whereas the value of 186.7 mg/l at  $25\text{ }^{\circ}\text{C}$  has been mentioned by Crookes and Howe (1991).

#### **Partition Coefficient**

The partition coefficient (Pow) is defined as the ratio of the equilibrium concentrations of a dissolved substance in a two phase system consisting of two largely immiscible solvents. In the case of n-octanol and water:

$$\text{Pow} = \text{equilibrium } c_{\text{n-octanol}} : \text{equilibrium } c_{\text{water}}$$

The partition coefficient therefore is the quotient of two concentrations and is usually given in the form of its logarithm to base ten ( $\log\text{Pow}$ ).

The logPow value at 25 °C was determined to be 3.13 by Tewari et al. (1982). This value was used for further calculations because the exact testing temperature was given. But nevertheless the value of 3.15 mentioned by Crookes and Howe (1991) and Verschueren (1983) correspond very well.

Table 1.1 Summary of physico-chemical properties

| Property   | Value                                |                       |
|--|--------------------------------------|-----------------------|
| Physical state                                       | liquid at 25 °C                      |                       |
| Melting point  | - 94.949 °C                          | Gerhartz (1987)       |
| Boiling point (at 1013 hPa)                          | 136.186 °C                           | Gerhartz (1987)       |
| Relative density                                     | 0.8670 at 20 °C                      | Lide (1991-1992)      |
| Vapour pressure                                      | p(20 °C) = 9.3 hPa                   | Auer Technikum (1988) |
| Water solubility                                     | 160 mg/l at 25 °C                    | Lide (1991-1992)      |
| Partition coefficient<br>n-octanol/water (log value) | 3.13 at 25 °C                        | Tewari et al. (1983)  |
| Granulometry   | not applicable (liquid)              |                       |
| Conversion factors                                   |                                      |                       |
| Flash point  | 23 °C                                | CHEMSAFE              |
| Autoflammability                                     | 430 °C                               | CHEMSAFE              |
| Flammability   | highly flammable                     | CHEMSAFE              |
| Explosive properties                                 | not explosive                        | CHEMSAFE              |
| Oxidizing properties                                 | not oxidizing<br>(structure)         |                       |
| Viscosity  |                                      |                       |
| Henry's constant                                     | 617 Pa m <sup>3</sup> /mol           | calculated            |
| Surface tension                                      | 28.48 mN/m                           | Gerhartz (1987)       |
| Index of refraction (nd)                             | 1.49588 at 20 °C<br>1.49320 at 25 °C | Gerhartz (1987)       |



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## 2 MANUFACTURE AND USES

See Risk Assessment Report

## 3 CLASSIFICATION AND LABELLING

### 3.1 Classification in Annex I of Directive 67/548/EEC

(Classification according to Annex I of the directive 67/548/EEC)

|         |      |                       |
|---------|------|-----------------------|
| F       | R 11 | Highly flammable      |
| Harmful | R 20 | Harmful by inhalation |

#### Proposal of the rapporteur

The entry in Annex I of directive 67/548/EEC does not yet include all categories of danger and qualifying risk phrases that have to be assigned according to the data presented. It is therefore proposed to amend the entry. The substance should be classified and labeled **additionally** with:

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|            |  |
|------------|--|
| R 36/37/38 | Irritating to eyes, respiratory tract and to skin                                    |
| R48/20     | Harmful: Danger of serious damage to health by prolonged exposure through inhalation |
| R 65       | Harmful: May cause lung damage if swallowed  |

Proposed classification based on GHS classification

H319 Eye Irrit.2  
H335 STOT Single3  
H315 Skin Irrit.2  
H373 STOT Rep.2  
H304 Asp.Tox.1

**3.2 Self classification(s)**

**4 ENVIRONMENTAL FATE PROPERTIES**

See Risk Assessment Report Draft of November 2008.

**5 HUMAN HEALTH HAZARD ASSESSMENT**

See Risk Assessment Report Draft of November 2008.

**6 HUMAN HEALTH HAZARD ASSESSMENT OF PHYSICO-CHEMICAL PROPERTIES**

See Risk Assessment Report Draft of November 2008.

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**7 ENVIRONMENTAL HAZARD ASSESSMENT**

See Risk Assessment Report Draft of November 2008.

**8 PBT AND VPVB ASSESSMENT**

**9 EXPOSURE ASSESSMENT**

See Risk Assessment Report Draft of November 2008.

**10 RISK CHARACTERISATION**

See Risk Assessment Report Draft of November 2008.

**INFORMATION ON ALTERNATIVES**

**11 INFORMATION ON THE RISKS TO HUMAN HEALTH AND THE ENVIRONMENT RELATED TO THE MANUFACTURE OF USE OF THE ALTERNATIVES**

**12 AVAILABILITY OF ALTERNATIVE, INCLUDING THE TIME SCALE**

**13 TECHNICAL AND ECONOMICAL FEASIBILITY**

## **JUSTIFICATION FOR RESTRICTION AT COMMUNITY LEVEL**

### **14 JUSTIFICATION THAT ACTION IS REQUIRED ON THE COMMUNITY-WIDE BASIS**

None

Other measures see Risk Reduction Strategy.

### **15 JUSTIFICATION FOR THE PROPOSES RESTRICTION**

**15.1 Effectiveness**

**15.2 Practicality**

**15.3 Monitorability**

## **SOCIO ECONOMIC ASSESSMENT**

## **OTHER INFORMATION**

*It is suggested to include here information on any consultation which took place during the development of the dossier. This could indicate who was consulted and by what means, what comments (if any) were received and how these were dealt with. The data sources (e.g registration dossiers, other published sources) used for the dossier could also be indicated here.*

## **REFERENCES**

See Risk Assessment Report Draft of November 2008.



**ANNEX**

See Risk Assessment Report Draft of November 2008.

Risk Reduction Strategy Draft of November 2008