



9 December 2011

**Substance Name: Phenolphthalein**  
**EC Number: 201-004-7**  
**CAS Number: 77-09-8**

**SUPPORT DOCUMENT FOR IDENTIFICATION OF**

**PHENOLPHTHALEIN**

**AS A SUBSTANCE OF VERY HIGH CONCERN BECAUSE OF ITS  
CMR PROPERTIES**

## **NOTE**

During the public consultation, in accordance with Article 59 (4) of the REACH Regulation, on the proposed identification of phenolphthalein as a Substance of Very High Concern (SVHC) on the basis of its classification as carcinogen category 1B no comments were received objecting the conclusion that the substance meets criteria set out in Article 57(a). Therefore, in accordance with Article 59 (6), phenolphthalein has been included in the Candidate List by ECHA.

The present support document comprises Part I (Justification) of the Annex XV dossier for identification of phenolphthalein as SVHC on the basis of Article 57(a) of REACH.

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**Substance Name: Phenolphthalein**

**EC Number: 201-004-7**

**CAS number: 77-09-8**

- The substance is identified as meeting the criteria of Article 57 (a) of Regulation (EC) 1907/2006 (REACH) owing to its classification as carcinogen category 1B<sup>1</sup>, which corresponds to classification as carcinogen category 2<sup>2</sup>.

### **Summary of how the substance(s) meet(s) the CMR (1A or 1B) criteria**

Phenolphthalein is listed by Index number 604-076-00-1 in Regulation (EC) No 1272/2008 and classified in Annex VI, Part 3, Table 3.1 (list of harmonised classification and labelling of hazardous substances) as carcinogen 1B<sup>3</sup> (H350: “May cause cancer.”). The corresponding classification in Annex VI, part 3, Table 3.2 (the list of harmonised classification and labelling of hazardous substances from Annex I to Directive 67/548/EEC) of Regulation (EC) No 1272/2008 is carcinogen category 2 (R45: “May cause cancer.”).

Therefore, this classification of phenolphthalein in Regulation (EC) No 1272/2008 shows that the substance meets the criteria for classification as carcinogen in accordance with Article 57 (a) of REACH.

**Registration dossiers submitted for the substance? Yes**

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<sup>1</sup> Classification in accordance with Regulation (EC) No 1272/2008 Annex VI, part 3, Table 3.1 List of harmonised classification and labelling of hazardous substances.

<sup>2</sup> Classification in accordance with Regulation (EC) No 1272/2008, Annex VI, part 3, Table 3.2 List of harmonised classification and labelling of hazardous substances (from Annex I to Council Directive 67/548/EEC).

<sup>3</sup> The classification of Carc 1A currently given in the specific concentration limits column in Annex VI, Part 3, Table 3.1 is erroneous and should read Carc 1B. This entry is included in the correcting act to the 1st ATP to CLP and will be active after its publication in the OJ – planned for first half of 2012.

## JUSTIFICATION

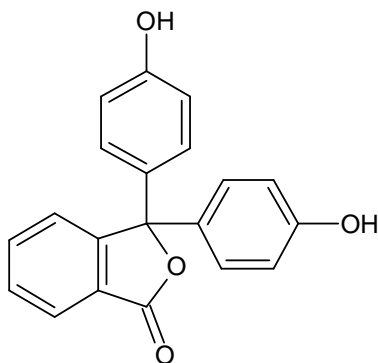
### 1 IDENTITY OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

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

**Table 1: Substance identity**

<b>EC number:</b>	201-004-7
<b>EC name:</b>	phenolphthalein
<b>CAS number (in the EC inventory):</b>	77-09-8
<b>CAS number:</b>	77-09-8
<b>Alternate CAS number:</b>	5768-87-6
<b>Deleted CAS numbers:</b>	467-29-8; 57214-20-7; 390417-24-0; 546094-13-7
<b>CAS name:</b>	1(3H)-Isobenzofuranone, 3,3-bis(4-hydroxyphenyl)-
<b>IUPAC name:</b>	3,3-Bis(4-hydroxyphenyl)-2-benzofuran-1(3H)-one
<b>Index number in Annex VI of the CLP Regulation</b>	604-076-00-1
<b>Molecular formula:</b>	C <sub>20</sub> H <sub>14</sub> O <sub>4</sub>
<b>Molecular weight:</b>	318.3 g/mol
<b>Synonyms:</b>	3,3-Bis(p-hydroxyphenyl)phthalide 3,3-Bis(4-hydroxyphenyl)phthalide 3,3-Bis(4-hydroxyphenyl)-1(3H)-isobenzofuranone

#### Structural formula:



## 1.2 Composition of the substance

**Name:** Phenolphthalein

**Description:** not relevant

**Degree of purity:**  $\geq 98\%$

**Table 2: Constituents**

Constituents	Typical concentration	Concentration range	Remarks
Phenolphthalein EC number: 201-004-7		$\geq 98.0\%$	Based on the received registration dossiers

**Table 3: Impurities**

Impurities	Typical concentration	Concentration range	Remarks
Unknown impurities		$\leq 2.0\%$	Based on the received registration dossiers

**Table 4: Additives**

Additives	Typical concentration	Concentration range	Remarks
None			Based on the received registration dossiers

## 1.3 Physico-chemical properties

**Table 5: Overview of physicochemical properties**

Property	Value	References
Physical state at 20°C and 101.3 kPa	Solid White or yellowish white minute, triclinic crystals	O'Neil, Maryadele J.; The Merck Index; Merck & Co Inc.; Whitehouse Station, NJ, USA; 14th Edition; 2006
Melting/freezing point	262.5 °C	Lide, David R.; CRC Handbook of Chemistry and Physics; CRC Press; Boca Raton, London, New York; 88th Edition; 2007-2008
Boiling point	> 450 °C at 1013 hPa	Based on the received registration dossiers
Density	1.277 g/cm <sup>3</sup> at 25 °C	Lide, David R.; CRC Handbook of Chemistry and Physics; CRC Press; Boca Raton, London, New York; 88th Edition; 2007-2008
Vapour pressure (p)	< 0.001 Pa at 20 °C	Based on the received registration dossiers
Water solubility	3.36 mg/l at 20 °C	Based on the received registration dossiers
Partition coefficient n-octanol/water (log value)	2.4 at pH 7.4	O'Neil, Maryadele J.; The Merck Index; Merck & Co Inc.; Whitehouse Station, NJ, USA; 14th Edition; 2006
Dissociation constant (pKa)	9.7 at 25 °C	O'Neil, Maryadele J.; The Merck Index; Merck & Co Inc.; Whitehouse Station, NJ, USA; 14th Edition; 2006

## 2 HARMONISED CLASSIFICATION AND LABELLING

**Table 6: Classification according to Annex VI, Part 3, Table 3.1 (list of harmonised classification and labelling of hazardous substances) of Regulation (EC) No 1272/2008**

Index No	International Chemical Identification	Classification		Labelling			Spec. Conc. Limits, M-factors	Notes
		Hazard Class and Category Code(s)	Hazard statement code(s)	Pictogram Signal Word Code(s)	Hazard statement code(s)	Suppl. Hazard statement code(s)		
604-076-00-1	phenolphthalein	Carc. 1B Muta. 2 Repr. 2	H350 H341 H361f***	GHS08 Dgr	H350 H341 H361f***		Carc. 1B <sup>1)</sup> H350: C ≥ 1 %	

<sup>1)</sup> The classification of Carc 1A currently given in the specific concentration limits column in Annex VI, Part 3, Table 3.1 is erroneous and should read Carc 1B. This entry is included in the correcting act to the 1st ATP to CLP and will be active after its publication in the OJ – planned for first half of 2012.

**Table 7: Classification according to Annex VI, Part 3, Table 3.2 (list of harmonized classification and labelling of hazardous substances from Annex I of Council Directive 67/548/EEC) of Regulation (EC) No 1272/2008**

Index No	International Chemical Identification	Classification	Labelling	Concentration Limits	Notes
604-076-00-1	phenolphthalein	Carc. Cat. 2; R45 Muta. Cat. 3; R68 Repr. Cat. 3; R62	T R: 45-62-68 S: 53-45	Carc. Cat. 2; R45: C ≥ 1 %	



### **3 ENVIRONMENTAL FATE PROPERTIES**

*Not relevant for the identification of the substance as SVHC in accordance with Article 57(a).*

### **4 HUMAN HEALTH HAZARD ASSESSMENT**

*Not relevant for the identification of the substance as SVHC in accordance with Article 57(a).*

### **5 ENVIRONMENTAL HAZARD ASSESSMENT**

*Not relevant for the identification of the substance as SVHC in accordance with Article 57(a).*

## **6 CONCLUSIONS ON THE SVHC PROPERTIES**

### **6.1 PBT, vPvB assessment**

Not relevant.

### **6.2 CMR assessment**

Phenolphthalein is listed by Index number 604-076-00-1 in Regulation (EC) No 1272/2008 and classified in Annex VI, Part 3, Table 3.1 (list of harmonised classification and labelling of hazardous substances) as carcinogen, Carc. 1B<sup>4</sup> (H350: “May cause cancer.”). The corresponding classification in Annex VI, part 3, Table 3.2 (the list of harmonised classification and labelling of hazardous substances from Annex I to Directive 67/548/EEC) of Regulation (EC) No 1272/2008 is carcinogen category 2 (R45: “May cause cancer.”).

Therefore, this classification of phenolphthalein in Regulation (EC) No 1272/2008 shows that the substance meets the criteria for classification as carcinogen in accordance with Article 57 (a) of REACH.

### **6.3 Substances of equivalent level of concern assessment**

Not relevant.

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<sup>4</sup> The classification of Carc 1A currently given in the specific concentration limits column in Annex VI, Part 3, Table 3.1 is erroneous and should read Carc 1B. This entry is included in the correcting act to the 1st ATP to CLP and will be active after its publication in the OJ – planned for first half of 2012.