

**Substance Name: 1,2-Benzenedicarboxylic acid, di-C6-10-alkyl esters; 1,2-Benzenedicarboxylic acid, mixed decyl and hexyl and octyl diesters with  $\geq 0.3\%$  of dihexyl phthalate (EC No. 201-559-5)**

**EC Number: 271-094-0, 272-013-1**

**CAS Number: 68515-51-5, 68648-93-1**

**MEMBER STATE COMMITTEE**

**SUPPORT DOCUMENT FOR IDENTIFICATION OF**

**1,2-BENZENEDICARBOXYLIC ACID, DI-C6-10-ALKYL ESTERS; 1,2-BENZENEDICARBOXYLIC ACID, MIXED DECYL AND HEXYL AND OCTYL DIESTERS WITH  $\geq 0.3\%$  OF DIHEXYL PHTHALATE (EC NO. 201-559-5)**

**AS SUBSTANCES OF VERY HIGH CONCERN BECAUSE OF THEIR CMR<sup>1</sup> PROPERTIES**

**Adopted on 29 May 2015**

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<sup>1</sup> CMR means carcinogenic, mutagenic or toxic for reproduction

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**Substance Names:** 1,2-benzenedicarboxylic acid, di-C6-10-alkyl esters<sup>2</sup>;  
1,2-benzenedicarboxylic acid, mixed decyl and hexyl and octyl diesters<sup>3</sup>

**EC Numbers:** 271-094-0, 272-013-1

**CAS numbers:** 68515-51-5, 68648-93-1

- The substances are identified as substances meeting the criteria of Article 57 (c) of Regulation (EC) No 1907/2006 (REACH) owing to their classification in the hazard class reproductive toxicity category 1B<sup>4</sup>.

### **Summary of how the substances meet the criteria set out in Article 57 of the REACH Regulation**

*1,2-Benzenedicarboxylic acid, di-C6-10-alkyl esters (EC No. 271-094-0); 1,2-benzenedicarboxylic acid, mixed decyl and hexyl and octyl diesters (EC No. 272-013-1) with  $\geq$  0.3% of dihexyl phthalate (EC No. 201-559-5),* meet the criteria of Article 57 (c) of Regulation (EC) 1907/2006 (REACH) owing to their classification as Repr. 1B (H360FD: May damage fertility. May damage the unborn child). This is due to the fact that dihexyl phthalate is covered by Index number 607-702-00-1 in part 3 of Annex VI to the CLP Regulation, and that no specific concentration limits are set in Annex VI of the CLP Regulation and therefore the generic concentration limit is to be used for the purpose of determining the classification of substances (or mixtures) containing dihexyl phthalate.

Therefore, this classification of *1,2-benzenedicarboxylic acid, di-C6-10-alkyl esters (EC No. 271-094-0); 1,2-benzenedicarboxylic acid, mixed decyl and hexyl and octyl diesters (EC No. 272-013-1) with  $\geq$  0.3% of dihexyl phthalate (EC No. 201-559-5)* shows that they meet the criteria for classification in the hazard class:

- reproductive toxicity category 1B in accordance with Article 57 (c) of REACH.

### **Registration dossiers submitted for the substances:**

**Yes, for EC No. 271-094-0.**

**No, for EC No. 272-013-1.**

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<sup>2</sup> The substances are identified as SVHC only where they contain  $\geq$  0.3 % (wt/wt) of dihexyl phthalate (EC No. 201-559-5).

<sup>3</sup> The substances are identified as SVHC only where they contain  $\geq$  0.3 % (wt/wt) of dihexyl phthalate (EC No. 201-559-5).

<sup>4</sup> Classification in accordance with section 3 of Annex I to Regulation (EC) No 1272/2008.

## 1. Identity of the substances and physical and chemical properties

### 1.1. Name and other identifiers of the substances

**Table 1: Substance identity**

<b>EC number:</b>	271-094-0	272-013-1
<b>EC name:</b>	1,2-Benzenedicarboxylic acid, di-C6-10-alkyl esters	1,2-Benzenedicarboxylic acid, mixed decyl and hexyl and octyl diesters
<b>CAS number (in the EC inventory):</b>	68515-51-5	68648-93-1
<b>CAS number:</b> <b>Deleted CAS numbers:</b>	-	-
<b>CAS name:</b>	1,2-Benzenedicarboxylic acid, di-C6-10-alkyl esters	1,2-Benzenedicarboxylic acid, mixed decyl and hexyl and octyl diesters
<b>IUPAC name:</b>	Di-C <sub>6-10</sub> alkyl phthalate	Di-C <sub>6-10</sub> (even numbered) alkyl phthalate
<b>Index number in Annex VI of the CLP Regulation</b>	-	-
<b>Molecular formula:</b>	Unspecified	Unspecified
<b>Molecular weight range:</b>	Unspecified	Unspecified
<b>Synonyms:</b>	Di(C6-C10)alkyl phthalate Phthalic acid, di(C6-C10)-alkyl esters Linear610Phthalate Esterification of phthalic anhydride and C6-10-alcohol	Esterification of phthalic anhydride and hexanol, octanol and decanol

The EC inventory entry for "1,2-benzenedicarboxylic acid, di-C6-10-alkyl esters" (EC number 271-094-0; CAS number 68515-51-5) has normally been considered for the purpose of EINECS as covering both the substance presenting even carbon numbers (i.e. C6, C8 and C10) and the substance presenting both the odd and even numbers (i.e. C6, C7, C8, C9, C10). This essentially comes from the conventions followed by the CAS Registry which do not make this further distinction on the presence or absence of odd numbers in alkyl descriptors such as "C6-10".

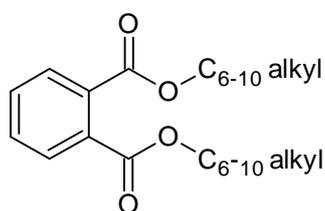
The EC inventory entry for "1,2-benzenedicarboxylic acid, mixed decyl and hexyl and octyl diesters" (EC number 272-013-1; CAS number 68648-93-1) on the other hand makes this distinction by defining the alkyl groups by their chemical name (i.e. hexyl, octyl and decyl) instead of the carbon range. This EC entry therefore covers the

substance with even carbon numbers, i.e. the substance "1,2-benzenedicarboxylic acid, di-C6-10 (even numbered)-alkyl esters" also known as "di-C<sub>6-10</sub> (even numbered) alkyl phthalate".

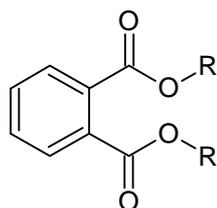
Both the substance with even carbon numbers and the substance with even and odd carbon numbers are within the scope of this proposal.

It should be noted that both EC inventory entries describe dialkyl phthalates presenting linear alkyl structures.

### Structural formula:



EC No. 271-094-0



EC No. 272-013-1

R= decyl, hexyl or octyl

## 1.2. Composition of the substance

**Name:** 1,2-benzenedicarboxylic acid, di-C6-10-alkyl esters<sup>5</sup>;

1,2-benzenedicarboxylic acid, mixed decyl and hexyl and octyl diesters<sup>6</sup>

**Description:** The substance "1,2-benzenedicarboxylic acid, di-C6-10-alkyl esters" should have a composition that is equivalent to the result from the diesterification reaction between 1,2-benzenedicarboxylic acid and "C6-10 alcohols". In line with the OECD Guidance for characterising oleochemical substances for assessment purposes (Series on Testing & Assessment No. 193, 2014), the upper concentration level in C6, C7, C8, C9 and C10 within the alcohols of "C6-10 alcohols" is normally expected to be  $\geq 10\%$  and  $< 80\%$ .

Any substance having a composition equivalent to the diesterification reaction products between 1,2-benzenedicarboxylic acid and "C6-10 alcohols" is within the scope of this proposal. This proposal is therefore not limited to substances obtained by reacting 1,2-

<sup>5</sup> with  $\geq 0.3\%$  (wt/wt) of dihexyl phthalate (EC No. 201-559-5).

<sup>6</sup> with  $\geq 0.3\%$  (wt/wt) of dihexyl phthalate (EC No. 201-559-5).

benzenedicarboxylic acid and "C6-10 alcohols" but covers also substances obtained from precursors such as phthalic anhydride instead of 1,2-benzenedicarboxylic acid.

Similarly, the substance named "1,2-benzenedicarboxylic acid, di-C6-10 (even numbered) alkyl esters" or "1,2-benzenedicarboxylic acid, mixed decyl and hexyl and octyl diesters" should have a composition that is equivalent to the result from the diesterification reaction between 1,2-benzenedicarboxylic acid and "C6-10 (even numbered) alcohols". The upper concentration level in C6, C8 and C10 within the alcohols of "C6-10 (even numbered) alcohols" is expected to be  $\geq 10\%$  and  $< 80\%$ .

Any substance having a composition equivalent to the diesterification reaction products between 1,2-benzenedicarboxylic acid and "C6-10 (even numbered) alcohols" is within the scope of this proposal. This proposal is therefore not limited to substances obtained by reacting 1,2-benzenedicarboxylic acid and "C6-10 (even numbered) alcohols" but covers also substances obtained from precursors such as phthalic anhydride instead of 1,2-benzenedicarboxylic acid.

### **1.3. Identity and composition of degradation products/metabolites relevant for the SVHC assessment**

Not relevant for the identification of the substances as SVHCs in accordance with Article 57 (c).

### **1.4. Identity and composition of structurally related substances (used in a grouping or read-across approach)**

Not relevant for the identification of the substances as SVHCs in accordance with Article 57 (c).

### **1.5. Physicochemical properties**

Not relevant for the identification of the substances as SVHCs in accordance with Article 57 (c).

## **2. Harmonised classification and labelling**

*1,2-Benzenedicarboxylic acid, di-C6-10-alkyl esters (EC No. 271-094-0); 1,2-benzenedicarboxylic acid, mixed decyl and hexyl and octyl diesters (EC No. 272-013-1)* are not themselves listed in Annex VI of Regulation (EC) No 1272/2008. Potential possibilities for harmonised classification of the substances themselves or their constituents could be dealt with in other processes than SVHC-identification.

According to Article 10(1) of the CLP Regulation, specific concentration limits and generic concentration limits are limits assigned to a substance indicating a threshold at or above which the presence of that substance in another substance (or in a mixture) as an identified impurity, additive or individual constituent leads to the classification of the substance (or mixture) as hazardous.

For dihexyl phthalate (EC No. 201-559-5) no specific concentration limits are set in Annex VI of the CLP Regulation and therefore the generic concentration limit is to be used for the purpose of determining classification of substances (or mixtures) containing dihexyl phthalate.

The generic concentration limit for reprotoxic substances, Repr. 1B, is 0.3 %, as set out in Table 3.7.2 in Part 3 of Annex I to the CLP Regulation.

**Table 2: Classification of *dihexyl phthalate* (according to Annex VI, Table 3.1 (list of harmonised classification and labelling of hazardous substances) of Regulation (EC) No 1272/2008)**

Index No	International Chemical Identification	EC No.	CAS No.	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)		
607-702-00-1	Dihexyl phthalate	201-559-5	84-75-3	Repr. 1B	H360FD	GHS08 Dgr	H360FD	-	-	-

Therefore, on such basis, the classification of *1,2-benzenedicarboxylic acid, di-C6-10-alkyl esters; 1,2-benzenedicarboxylic acid, mixed decyl and hexyl and octyl diesters where they contain dihexyl phthalate  $\geq 0.3\%$*  is as seen in **Table 3**.

**Table 3: Classification of *1,2-benzenedicarboxylic acid, di-C6-10-alkyl esters; 1,2-benzenedicarboxylic acid, mixed decyl and hexyl and octyl diesters where they contain dihexyl phthalate  $\geq 0.3\%$*  according to Art. 10 and Table 3.7.2 in Part 3 of Annex I to Regulation (EC) No 1272/2008 (CLP Regulation), on the basis of the entry with index number for dihexyl phthalate in Part 3 of Annex VI to CLP Regulation**

Index No	International Chemical Identification	EC No.	CAS No.	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)		
	1,2-benzenedicarboxylic acid, di-C6-10-alkyl esters with dihexyl phthalate $\geq 0.3\%$	271-094-0	6851-51-5	Repr. 1B	H360FD	GHS08 Dgr	H360FD	-	-	-
	1,2-benzenedicarboxylic acid, mixed decyl and hexyl and octyl diesters with dihexyl phthalate $\geq 0.3\%$	272-013-1	6864-893-1	Repr. 1B	H360FD	GHS08 Dgr	H360FD	-	-	-

H360FD = May damage fertility. May damage the unborn child.

### 3. Environmental fate properties

Not relevant for the identification of the substances as SVHCs in accordance with Article 57 (c) REACH.

### 4. Human health hazard assessment

Not relevant for the identification of the substances as SVHCs in accordance with Article 57 (c) REACH.

### 5. Environmental hazard assessment

Not relevant for the identification of the substances as SVHCs in accordance with Article 57 (c) REACH.

## 6. Conclusions on the SVHC Properties

### 6.1. CMR assessment

*1,2-Benzenedicarboxylic acid, di-C6-10-alkyl esters (EC No. 271-094-0); 1,2-benzenedicarboxylic acid, mixed decyl and hexyl and octyl diesters (EC No. 272-013-1) with  $\geq$  0.3% of dihexyl phthalate (EC No. 201-559-5),* meet the criteria of article 57 (c) of Regulation (EC) 1907/2006 (REACH) owing to their classification as Repr. 1B (H360FD: May damage fertility. May damage the unborn child). This is due to the fact that dihexyl phthalate is covered by Index number 607-702-00-1 in part 3 of Annex VI to the CLP Regulation, and that no specific concentration limits are set in Annex VI of the CLP Regulation and therefore the generic concentration limit is to be used for the purpose of determining the classification of substances (or mixtures) containing dihexyl phthalate.

Therefore, this classification of *1,2-benzenedicarboxylic acid, di-C6-10-alkyl esters (EC No. 271-094-0); 1,2-benzenedicarboxylic acid, mixed decyl and hexyl and octyl diesters (EC No. 272-013-1) with  $\geq$  0.3% of dihexyl phthalate (EC No. 201-559-5)* shows that they meet the criteria for classification in the hazard class:

- reproductive toxicity category 1B in accordance with Article 57 (c) of REACH.

## References

- (CLP). Regulation (EC) No 1272/2008 of the European Parliament and of the Council of 16 December 2008 on classification, labelling and packing of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006. Official Journal of the European Union, L353: 1-1355.
- ECHA Dissemination site (2015). [1,2-Benzenedicarboxylic acid, di-C6-10-alkyl esters](http://echa.europa.eu/information-on-chemicals/registered-substances). Information on registered substances, published on ECHA's website. <http://echa.europa.eu/information-on-chemicals/registered-substances>. Accessed 2015-01-28.
- ECHA Guidance for identification and naming of substances under REACH and CLP. Version: 1.3, February 2014 [http://echa.europa.eu/documents/10162/13643/substance\\_id\\_en.pdf](http://echa.europa.eu/documents/10162/13643/substance_id_en.pdf).
- OECD Guidance for characterising oleochemical substances for assessment purposes (Series on Testing & Assessment No. 193, 2014), [http://www.oecd.org/officialdocuments/publicdisplaydocumentpdf/?cote=env/jm/mono\(2014\)6&doclanguage=en](http://www.oecd.org/officialdocuments/publicdisplaydocumentpdf/?cote=env/jm/mono(2014)6&doclanguage=en)
- (REACH). Regulation (EC) No 1907/2006 of the European Parliament and of the Council of 18 December 2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH), establishing a European Chemicals Agency, amending Directive 1999/45/EC and repealing Council Regulation (EEC) No 793/93 and Commission Regulation (EC) No 1488/94 as well as Council Directive 76/769/EEC and Commission Directives 91/155/EEC, 93/67/EEC, 93/105/EC and 2000/21/EC. Official Journal of the European Union, L396: 1-849.