



Substance name:
**1,2-Benzenedicarboxylic acid, di-C7-11 –
branched and linear alkyl esters (DHNUP)**

EC number: 271-084-6
CAS number: 68515-42-4

**MEMBER STATE COMMITTEE
SUPPORT DOCUMENT FOR IDENTIFICATION OF**

**1,2-BENZENEDICARBOXYLIC ACID, DI-C7-11 BRANCHED AND
LINEAR ALKYL ESTERS (DHNUP)**

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

Adopted on 26 May 2011

CONTENTS

CONTENTS	2
JUSTIFICATION	4
1 Identity of the substance and physical and chemical properties	4
1.1 Name and other identifiers of the substance.....	4
1.2 Composition of the substance.....	5
1.3 Physico-chemical properties.....	5
2 Harmonised classification and labelling	6
3 Environmental fate properties.....	7
4 Human health hazard assessment	7
5 Environmental hazard assessment	7
6 Conclusions on the SVHC Properties.....	7
6.1 CMR assessment	7
REFERENCES	8

TABLES

Table 1: Substance identity.....	5
Table 2: Overview of physicochemical properties	7
Table 3: Classification according to part 3 of Annex VI, Table 3.1 ((list of harmonised classification and labelling of hazardous substances) of Regulation (EC) No 1272/2008	8
Table 4: Classification according to part 3 of Annex VI, 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.....	8

LIST OF ABBREVIATIONS

CMR	Carcinogenic, Mutagenic or toxic to Reproduction
PBT	Persistent, Bioaccumulative and Toxic
SVHC	Substance of Very High Concern
vPvB	very Persistent and very Bioaccumulative

Substance name: 1,2-Benzenedicarboxylic acid, di-C₇₋₁₁ -branched and linear alkyl esters (DHNUP)

EC number: 271-084-6

CAS number: 68515-42-4

- The substance is identified as a substance meeting the criteria of Article 57(c) of Regulation (EC) No 1907/2006 (REACH) owing to its classification as toxic for reproduction 1B¹, which corresponds to classifications as toxic for reproduction category 2².

Summary of how the substance meets the CMR (1A or 1B) criteria

DHNUP (1,2-Benzenedicarboxylic acid, di-C₇₋₁₁ -branched and linear alkyl esters) is listed by Index number 607-480-00-6 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 toxic for reproduction, Repr. 1B (H360Df: “May damage the unborn child. Suspected of damaging fertility). 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 toxic for reproduction category 2 (R61: “May cause harm to the unborn child”).

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

Registration dossiers submitted for the substance: No

¹ 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.

² 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).

JUSTIFICATION

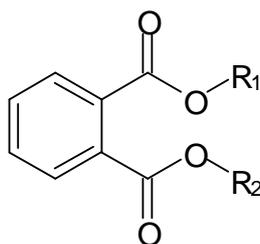
1 IDENTITY OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

1.1 Name and other identifiers of the substance

Table 1: Substance identity

EC number:	271-084-6
EC name:	1,2-Benzenedicarboxylic acid, di-C7-11-branched and linear alkyl esters
CAS number (in the EC inventory):	68515-42-4
CAS number:	68515-42-4
CAS name:	1,2-Benzenedicarboxylic acid, di-C ₇₋₁₁ -branched and linear alkyl esters
IUPAC name:	Di-C7-11-(linear and branched)-alkyl phthalate
Index number in Annex VI of the CLP Regulation	607-480-00-6
Molecular formula:	C ₂₂ H ₃₄ O ₄ -C ₃₀ H ₅₀ O ₄
Molecular weight range:	362 – 474
Synonyms:	Dialkyl phthalate (C ₇₋₁₁) branched and linear phthalate ester; 711P; D711P; Di-711-phthalate; Dialkyl(C ₇₋₁₁ -branched and linear) phthalate; Di(heptyl, nonyl, undecyl) phthalate (DHNUP); Di(heptyl, nonyl, undecyl) phthalate (mixed isomers); Phthalic acid, dialkyl (C7-C11) ester; Santicizer 711 ³

³ [Environment Canada 2009]

Structural formula:

R_1 and R_2 can be linear or branched

1.2 Composition of the substance

This substance is a UVCB (Unknown or Variable Composition, Complex Reaction Products, or Biological Materials), and may thus be characterized by a variety of structures. The formula given in section 1.1 represents a representative chemical formula and a general chemical formula (minimum to maximum number of atoms)

1.3 Physico-chemical properties**Table 2: Overview of physicochemical properties**

Property	Value	Remarks
Physical state at 20°C and 101.3 kPa	<i>Liquid</i>	<i>IUCLID dataset- [ECB 2000]*</i>
Melting/freezing point	<i>-57 °C (pour point)</i>	<i>IUCLID dataset- [ECB 2000]*</i>
Boiling point	<i>235-278 °C at 7 hPa</i>	<i>IUCLID dataset- [ECB 2000]*</i>
Vapour pressure	<i><10 Pa at 20 °C</i>	<i>IUCLID dataset- [ECB 2000]*</i>
Water solubility	<i>0.1 mg/L at 20 °C pH neutral</i>	<i>IUCLID dataset- [ECB 2000]*</i>
Partition coefficient n-octanol/water (log value)	<i>ca. 4.8</i>	<i>IUCLID dataset- [ECB 2000]*</i>
Dissociation constant	<i>No data</i>	<i>IUCLID dataset- [ECB 2000]*</i>
Density	<i>969-973 kg/m³ at 20 °C</i>	<i>IUCLID dataset- [ECB 2000]*</i>

* According to [Environment Canada 2009] the physico-chemical properties are based on a test chemical named Palatinol[®] 711P, a trade name representing the following six CAS Numbers: 85507-79-5, 68515-44-6, 68515-45-7, 111381-89-6, 111381-90-9 and 111381-91-0. It is notable that one of the components of DHNUP, diundecyl phthalate, (CAS No. 3648-20-2), is replaced by diundecyl phthalate, branched and linear (CAS No. 85507-79-5), in Palatinol[®] 711P. The IUCLID dataset, however, does not mention Palatinol[®] 711P in this context, and gives the impression that test results is based on experiments with DHNUP (CAS No 68515-42-4). [Environment Canada 2009] has in their assessment considered Palatinol[®] 711P to be equivalent to DHNUP

2 HARMONISED CLASSIFICATION AND LABELLING

DHNUP (1,2-Benzenedicarboxylic acid, di-C₇₋₁₁ -branched and linear alkyl esters) is listed by Index number 607-480-00-6 in Regulation (EC) No 1272/2008 as follows:

Table 3: Classification according to part 3 of 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	Classification *1		Labelling			Specific 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)		
607-480-00-6	1,2-Benzenedicarboxylic acid, di-C ₇₋₁₁ -branched and linear alkyl esters	Repr. 1B	H360Df	GHS08 Dgr	H360Df	H360Df		

Hazards statement code: H360Df: May damage the unborn child. Suspected of damaging fertility.

Table 4: Classification according to part 3 of Annex VI, 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
607-480-00-6	1,2-Benzenedicarboxylic acid, di-C ₇₋₁₁ -branched and linear alkyl esters	Repr. Cat. 2; R61 Repr. Cat. 3; R62	T R: 61-62 S: 53-45		

3 ENVIRONMENTAL FATE PROPERTIES

Not relevant for this dossier.

4 HUMAN HEALTH HAZARD ASSESSMENT

See section 2 on Harmonised Classification and Labelling.

5 ENVIRONMENTAL HAZARD ASSESSMENT

Not relevant for this dossier.

6 CONCLUSIONS ON THE SVHC PROPERTIES

6.1 PBT, vPvB assessment

Not relevant for this dossier.

6.2 CMR assessment

DHNUP (1,2-Benzenedicarboxylic acid, di-C7-11 -branched and linear alkyl esters) is listed by Index number 607-480-00-6 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 toxic for reproduction, Repr. 1B (H360Df: “May damage the unborn child. Suspected of damaging fertility). 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 toxic for reproduction category 2 (R61: “May cause harm to the unborn child”).

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

6.3 Substances of equivalent level of concern assessment

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

REFERENCES

ECB 2000. IUCLID dataset for 1,2-Benzenedicarboxylic acid, di-C₇₋₁₁-branched and lineal alkyl esters (CAS 68515-42-4). <http://ecb.jrc.it/iuclid-datasheet/68515424.pdf>

Environment Canada 2009. Screening Assessment for the challenge. 1,2-Benzenedicarboxylic acid, di-C₇₋₁₁-branched and lineal alkyl esters. CAS 68515-42-4.