

Annex XV dossier

**PROPOSAL FOR IDENTIFICATION OF A SUBSTANCE AS A
CMR CAT 1A OR 1B, PBT, vPvB OR A SUBSTANCE OF AN
EQUIVALENT LEVEL OF CONCERN**

Substance Name(s): n-Pentyl-isopentyl phthalate

EC Number(s): -

CAS Number(s): 776297-69-9

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Substance Name(s): n-Pentyl-isopentyl phthalate

EC Number(s): -

CAS number(s): 776297-69-9

- The substance is proposed to be identified as substance meeting the criteria of Article 57 (c) of Regulation (EC) 1907/2006 (REACH) owing to its classification as toxic for reproduction category 1B¹ which corresponds to classification as toxic for reproduction category 2².

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

n-Pentyl-isopentyl phthalate is listed by Index number 607-426-00-1 of 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 (H360FD: “May damage fertility. May damage the unborn child.”). 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, Repr. Cat. 2 (R60-61;” May impair fertility. 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).

PART I

JUSTIFICATION

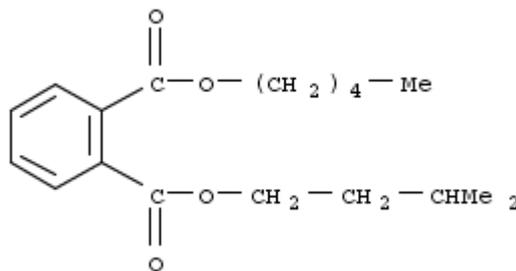
1 IDENTITY OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

1.1 Name and other identifiers of the substance

Table 1: Substance identity

EC number:	-
EC name:	-
CAS number (in the EC inventory):	-
CAS number:	776297-69-9
CAS name:	1,2-Benzenedicarboxylic acid, 1-(3-methylbutyl) 2-pentyl ester
IUPAC name:	n-Pentyl-isopentyl phthalate
Index number in Annex VI of the CLP Regulation	607-426-00-1
Molecular formula:	C ₁₈ H ₂₆ O ₄
Molecular weight range:	306 g/mol
Synonyms:	n-Pentyl-isopentyl phthalate 1,2-Benzenedicarboxylic acid, 3-methylbutyl pentyl ester

Structural formula:



1.2 Composition of the substance

Name: n-Pentyl-isopentyl phthalate

Description: mono constituent substance

Degree of purity: Registration dossiers or other information on concentration ranges are not available.

Table 2: Constituents

Constituents	Typical concentration	Concentration range	Remarks
n-Pentyl-isopentyl phthalate			

Table 3: Impurities

Impurities	Typical concentration	Concentration range	Remarks

Table 4: Additives

Additives	Typical concentration	Concentration range	Remarks

1.3 Physico-chemical properties

Table 5: Overview of physicochemical properties

Property	Value	Remarks
Physical state at 20°C and 101.3 kPa		
Melting/freezing point		
Boiling point		
Vapour pressure		
Water solubility		
Partition coefficient n-octanol/water (log value)		
Dissociation constant		
[enter other property, if relevant, or delete row]		

No physical and chemical properties could be found in well known databases (e.g. the recommended databases of Guidance on information requirements and chemical safety assessment

Chapter R.7a: Endpoint specific guidance). Furthermore no registration dossiers are available. Hence no physical and chemical properties could be given.

2 HARMONISED CLASSIFICATION AND LABELLING

n-Pentyl-isopentyl phthalate is listed by Index number 607-426-00-1 of 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 follows:

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	EC No	CAS No	Classification		Labelling	
				Hazard Class and Category Code(s)	Hazard statement code(s)	Pictogram, Signal Word Code(s)	Hazard statement code(s)
607-426-00-1	n-pentyl-isopentyl phthalate	-	-	Repr. 1B Aquatic Acute 1	H360FD H400	GHS08 GHS09 Dgr	H360FD H400

Hazard statement code: H360FD: May damage fertility. May damage the unborn child.

n-Pentyl-isopentyl phthalate is covered by Index number 607-426-00-1 of Regulation (EC) No 1272/2008 in Annex VI, Part 3, Table 3.2 (list of harmonised classification and labelling of hazardous substances from Annex I to Directive 67/548/EEC) as follows:

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

INDEX NO	CHEMICAL NAME	EC NO	CAS NO	CLASSIFICATION	LABELLING
607-426-00-1	n-pentyl-isopentyl phthalate			Repr. Cat. 2; R60-61 N; R50	T; N R: 60-61-50 S: 53-45-61

Risk phrases: R60-61: May impair fertility. May cause harm to the unborn child

3 ENVIRONMENTAL FATE PROPERTIES

Not relevant.

4 HUMAN HEALTH HAZARD ASSESSMENT

See section 2 on Harmonised Classification and Labelling.

5 ENVIRONMENTAL HAZARD ASSESSMENT

Not relevant.

6 CONCLUSIONS ON THE SVHC PROPERTIES

6.1 PBT, vPvB assessment

Not relevant.

6.2 CMR assessment

n-Pentyl-isopentyl phthalate is covered by Index number 607-426-00-1 of 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 (H360FD: “May damage fertility. May damage the unborn child.”). 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, Repr. Cat. 2 (R60-61;” May impair fertility. 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.

PART II

INFORMATION ON USE, EXPOSURE, ALTERNATIVES AND RISKS

1 INFORMATION ON MANUFACTURE, IMPORT/EXPORT AND USES – CONCLUSIONS ON EXPOSURE

1.1 Information on Manufacture, Import/Export and Uses

n-Pentyl-isopentyl phthalate was not pre-registered and is not registered according to recently performed searches in REACH-IT. However, it is possible that the substance could be registered at a later date. According to the information available on ECHA's website there have been 70 notifications to the C&L inventory (status on 01.08.2012)³. No information could be identified on current annual EU import/export volumes. Common databases (e.g. SPIN) were checked to identify information about tonnage and use. Due to their similar physico-chemical properties to other transitional phthalates of carbon backbone lengths of C4-C6 e.g. di-n-butyl phthalate and diisopentyl phthalate concerning for example density (Lide 1997) pentyl phthalates can be used as plasticisers in plastic material (Rein 1937, Schaeffler 2011). The substance has not been reported by EU Industry as an HPVC or LPVC according to previous existing substances regulation (ESIS). Therefore it can be assumed that n-pentyl-isopentyl phthalate is not manufactured in the Community or placed on the market in quantities of one tonne or more per year.

1.2 Information on Exposure

No measured data are available on n-pentyl-isopentyl phthalate exposure concentration at the workplace.

No information about concentrations of n-pentyl-isopentyl phthalate in consumer products is available. The presence/absence in house dust may indicate possible sources however no data about house dust measurements were identified. A current study of house dust measurements in kindergarten carried out by the German Federal Environment Agency (UBA) suggests that only low concentrations of n-pentyl-isopentyl phthalate can be expected (unpublished report, personal communication). Final results are not yet available.

A quantification of exposure is not possible due to a lack of data. It should be assumed that exposure if at all is very low.

³ <http://clp-inventory.echa.europa.eu/SummaryOfClassAndLabelling.aspx?SubstanceID=153493&HarmOnly=no?fc=true&lang=en>

2 CURRENT KNOWLEDGE ON ALTERNATIVES

The effects of phthalates on reproduction appear to be associated predominantly with the transitional phthalates of carbon backbone lengths of C4-C6. In general lower molecular weight phthalates (\leq C3) and higher molecular weight phthalates (\geq C7) appeared not to induce developmental effects (Phthalates Hazard Compendium, 2008). However it is noted that there may be exceptions from this general rule and it has to be kept in mind that some low and high molecular weight phthalates show effects at higher levels of exposure. Alternative substances might be phthalates with short or long carbon backbones, depending on the physicochemical property needed.

Depending on the functionality needed chemicals like citrates (biodegradable and not toxic), adipates, phosphates (resistant to ignition and burning), trimellitates (exceptional thermal properties), etc. could be used as alternatives of n-pentyl-isopentyl phthalate. Potential alternatives have been assessed in the case of bis(2-ethylhexyl)phthalate (DEHP, CAS No 117-81-7) and could also be of interest for replacing n-pentyl-isopentyl phthalate (ECHA, 2009).

3 RISK-RELATED INFORMATION

There are currently no registrations for n-pentyl-isopentyl phthalate. A risk characterisation is not possible due to a lack of information about possible exposure. However, it is possible that the substance could be registered at a later date. This probability is realistic because other phthalates are already included in the candidate list and/or banned from several uses. Based on its properties, functions and uses, n-pentyl-isopentyl phthalate might be considered as a possible substitute for already regulated phthalates. In this case, exposure to n-pentyl-isopentyl phthalate might arise. Possible substitution of hazardous phthalates by n-pentyl-isopentyl phthalate should be prevented by equal treatment of all phthalates classified as toxic to reproduction. Based on the inherent toxic properties and its classification n-pentyl-isopentyl phthalate represents a hazardous phthalate.

REFERENCES

References to Part I

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.

<http://eur-lex.europa.eu/LexUriServ/LexUriServ.do?uri=oj:l:2006:396:0001:0849:en:pdf>

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References to Part II

ECHA 2009. Data on manufacture, import, export, uses and releases of Bis(2-ethylhexyl)phthalate (DEHP) as well as information on potential alternatives to its use. The technical work on this report has been led by COWI A/S, supported by IOM and Entec UK Ltd under framework contract ECHA/2008/2.

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SPIN Database, 2012:

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