Substance Name: Diisopentylphthalate (DIPP)

EC Number: 210-088-4

CAS Number: 605-50-5

SUPPORT DOCUMENT FOR IDENTIFICATION OF

DIISOPENTYLPHTHALATE (DIPP)

AS A SUBSTANCE OF VERY HIGH CONCERN BECAUSE OF ITS CMR[1] PROPERTIES

[1] CMR means carcinogenic, mutagenic or toxic for reproduction

CONTENTS

TABLES

Substance Name(s): Diisopentylphthalate (DIPP)

EC Number(s): 210-088-4

CAS number(s): 605-50-5

The substance is 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 1B[2] which corresponds to classification as toxic for reproduction category 2[3].

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

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

Registration dossiers submitted for the substance? Yes

[2] 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, OJ L 353, p.1, 31.12.2008.

[3] 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), OJ L 353, p.1, 31.12.2008.

Justification

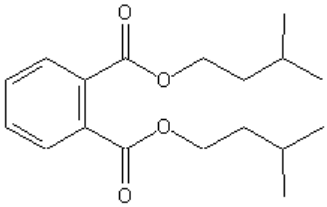
1 Identity of the substance and physical and chemical properties

1.1 Name and other identifiers of the substance

Table 1: Substance identity

EC number:	210-088-4
EC name:	diisopentylphthalate
CAS number (in the EC inventory):	605-50-5
CAS number:	605-50-5
CAS name:	1,2-benzenedicarboxylic acid, 1,2-bis(3-methylbutyl) ester
IUPAC name:	Bis(3-methylbutyl) 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:	306,40 g/mol
Synonyms:	1,2-Benzenedicarboxylic acid, bis(3-methylbutyl) ester Diisoamyl phthalate Isoamyl phthalate

Structural formula:



1.2 Composition of the substance

Name: Diisopentylphthalate

Description: clear slightly yellow liquid

Degree of purity: see confidential Annex II

1.3 Physico-chemical properties

Table 2: Overview of physico-chemical properties

Property	Value	Remarks
Physical state at 20°C and 101.3 kPa	*Clear liquid, slightly yellow*	*Registration data from dissemination database*[4]
Melting/freezing point	*Freezing point less than -25°C*	*Registration data from dissemination database*
Boiling point	*339°C*	*Registration data from dissemination database*
Vapour pressure	*0.025Pa at 25°C*	*Registration data from dissemination database*
Water solubility	*1.1mg/l at 20°C*	*Registration data from dissemination database*
Partition coefficient n-octanol/water (log P_{OW})	log P_{OW} *=5.6*	*Registration data from dissemination database*
Flashpoint	*166°C*	*Registration data from dissemination database*
Auto Flammability at 1013hPa	*>=400°C*	*Registration data from dissemination database*
Oxidising property	*No oxidising properties.*	*Registration data from dissemination database (QSAR)*
Density	1.02 g/cm³	*Registration data from dissemination database*

[4] http://apps.echa.europa.eu/registered/registered-sub.aspx

2 Harmonised classification and labelling

DIPP is covered by index number 607-426-00-1 in Annex VI, part 3 of Reg. (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	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)		
607-426-00-1	diisopentylphthalate	210-088-4	605-50-5	Repr. 1B Aquatic Acute 1	H360-FD H400	GHS08 GHS09 Dgr	H360FD H400			

Table 4: Classification according to part 3 of Annex VI, Table 3.2 (list of harmonised 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	EC No	CAS No	Classification	Labelling	Concentration Limits	Notes
607-426-00-1	diisopentylphthalate	210-088-4	605-50-5	Repr. Cat. 2; R60-61 N; R50	T; N R: 60-61-50 S: 53-45-61		

Self-classification:

According to registration information, the substance is additionally classified as Skin Sens. 1, H317.

For additional confidential information from the C&L inventory see Annex II Chapter 4.

3 Environmental fate properties

Not relevant.

4 Human health hazard assessment

See section 2 Harmonised Classification and Labelling and Supplementary Information in Annex I.

5 Environmental hazard assessment

Not relevant.

6 Conclusions on the SVHC Properties

6.1 PBT, vPvB assessment

Not relevant.

6.2 CMR assessment

Diisopentylphthalate (DIPP) 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(s) in Regulation (EC) No 1272/2008 shows that the substance 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.

7 REFERENCES

http://apps.echa.europa.eu/registered/registered-sub.aspx

ANNEX I

SUPPLEMENTARY INFORMATION ON THE LEADING HEALTH EFFECTS AND TOXICOKINETICS

1 Toxicokinetics (absorption, metabolism, distribution and elimination)

For the substance DIPP a good skin penetration potential can be expected as for the structurally-related diisobutyl phthalate about 10 % of the occlusively applied 30 mg dose was absorbed by rats within 24 h.

Absorption via the gastrointestinal tract is substantiated by systemic effects in animal experiments.

Alkyl phthalates are assumed to be absorbed via the respiratory tract. Since the vapor pressure is very low, inhalative exposure is only to be expected if DIPP is strongly heated or if aerosols are formed.

Studies regarding metabolism of DIPP are not available. Analogous to other medium-chained alkyl phthalates, it is to be expected that a hydrolysis to the monoester mono-isopentyl phthalate takes place in the liver, followed be subsequent formation of phthalic acid and methyl butanol. The elimination of these metabolites or consecutive products or conjugates probably proceeds with the urine and also in part with the faeces (GESTIS).

2 Toxicity for reproduction

2.1 Developmental toxicity

After oral administration of a mixture Di-n-pentylphthalate with di-iso-pentylphthalate to Wistar rats in doses of 40, 200 and 1,000 mg/kg from the 6th - 15th day of pregnancy (8 - 10 animals per group; preparation in olive oil) the following results were obtained:

In the top dose all fetuses were resorbed (100% post-implantation loss). Dams on the 20th day of pregnancy showed increases in absolute and relative liver weights together with reduced feed intake and reduced body weight gain. No connection can be seen between maternal and fetal effects. Relating the only slight maternal to the severe fetal effects, the fetal toxicity is regarded as specific and selective. No effects were observed at 200 and 40 mg/kg respectively (Hellwig et al., 1997; ECBI/65/00 Add 9).

Additional information:

According to Hannas, 2011 and earlier conducted studies (Foster, 1980) there is strong evidence that dipentylphthalate (CAS 131-18-0) is an equal or even more potent testicular toxicant than DEHP. This is likely to be valid also for other structurally related pentyl phthalates, like DIPP. This is supported by the results of the above mentioned study by Hellwig, 1997. The mixture of pentyl phthalates caused a 100% resorption at 1000mg/kg/day while DEHP caused malformations in 70% of the litters at the same dose.

2.2 Effects on fertility

There are no studies on fertility with DIPP available to date. A fertility reducing action is suspected because of the structural relationship to di-n-pentyl phthalate and dibutylphthalate and the findings available for these substances. The monoesters of phthalic acid esters of medium chain length (C4 – C6) cause damage to the germinal epithelium in the testis. Sertoli cells in the seminiferous tubules are the primary site of attack. They exhibit considerable vacuolization of the smooth endoplasmatic reticulum resulting in a reduced fertility. As a consequence the germinal epithelium may be lost. (GESTIS; BAuA, 2001; ECBI/65/00 Add2).