Annex XV report

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: 1,2-Benzenedicarboxylic acid, dihexyl ester, branched and linear

EC Number: 271-093-5

CAS Number: 68515-50-4

Submitted by: Swedish Chemicals Agency, Sweden

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Substance Name: 1,2-Benzenedicarboxylic acid, dihexyl ester, branched and linear

EC Number: 271-093-5

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- The substance is proposed to be identified as a substance meeting the criteria of Article 57 (c) of Regulation (EC) 1907/2006 (REACH)[1] owing to the adopted opinion[2] by the Committee for Risk Assessment (RAC) which has agreed that the substance meets the criteria for classification as toxic for reproduction category 1B according to Regulation (EC) No 1272/2008 (CLP)[3].

Summary of how the substance meets the CMR (Cat 1A or 1B), PBT or vPvB criteria, or is considered to be a substance giving rise to an equivalent level of concern

In accordance with Article 37(4) of the CLP Regulation, the Committee for Risk Assessment (RAC) has adopted an opinion for harmonised classification and labelling of *1,2-benzenedicarboxylic acid, dihexyl ester, branched and linear* in June 2013. At RAC-25 the RAC adopted the opinion that *1,2-benzenedicarboxylic acid, dihexyl ester, branched and linear* meets the criteria for classification as toxic for reproduction Repr. 1B, H360FD ("May damage fertility. May damage the unborn child."). The corresponding classification in accordance with Directive 67/548/EEC would be toxic for reproduction Repr. Cat.2, R60-61 ("May impair fertility. May cause harm to the unborn child."). After decision of the European Commission, confirming the classification as Repr. 1B, the new classification will be included in the list of harmonised classifications (Annex VI to the CLP Regulation).

Therefore, *1,2-benzenedicarboxylic acid, dihexyl ester, branched and linear* meets the criteria of Article 57(c) of Regulation (EC) 1907/2006 (REACH Regulation).

Registration dossier(s) submitted for the substance? No

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[1] 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.

[2] Committee for Risk Assessment RAC Opinion proposing harmonised classification and labelling at EU level of 1,2-Benzenedicarboxylic acid, dihexylester, branched and linear EC number: 271-093-5 CAS number: 68515-50-4 CLH-O-0000002695-67-03/F Adopted 7 June 2013 http://echa.europa.eu/documents/10162/18d3ed6d-91c5-48d0-844a-8383ab5723b3

[3] Regulation (EC) No 1272/2008 of the European Parliament and of the Council of 16 December 2008 on classification, labelling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006.

PART I

JUSTIFICATION

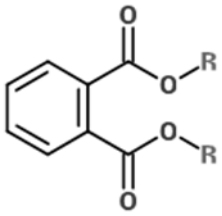
1 IDENTITY OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

1.1 Name and other identifiers of the substance

Table 1 Substance identity

EC number:	271-093-5
EC name:	1,2-Benzenedicarboxylic acid, dihexyl ester, branched and linear
CAS number (in the EC inventory):	68515-50-4
CAS number:	68515-50-4
CAS name:	1,2-Benzenedicarboxylic acid, 1,2-dihexyl ester, branched and linear
IUPAC name:	1,2-Benzenedicarboxylic acid, dihexyl ester, branched and linear
Index number in Annex VI of the CLP Regulation	-
Molecular formula:	$C_{20}H_{30}O_4$
Molecular weight range:	334 g/mol
Synonyms:	Dihexylphthalate, branched and linear Phthalic acid, dihexyl ester, branched and linear Dihexylphthalate, mixed isomers Phthalic anhydride, reaction products with hexanol, branched and linear Esterification of phthalic anhydride and hexanol, branched and linear

Structural formula:



R = C_6H_{13}, branched and linear

1.2 Composition of the substance

Name: 1,2-Benzenedicarboxylic acid, dihexyl ester, branched and linear

Description: UVCB substance

The CAS number 68515-50-4 represents a reaction product containing branched and/or linear isomers and/or combinations thereof. Two out of many possible isomers found in the UVCB substance *1,2-Benzenedicarboxylic acid, dihexyl ester, branched and linear* (CAS number 68515-50-4) are e.g. CAS number 71850-09-4 (di-isohexyl phthalate) and CAS number 84-75-3 (di-n-hexyl phthalate).

Typical concentrations and concentration ranges of the isomers in *1,2-benzenedicarboxylic acid, dihexyl ester, branched and linear* are not known.

1.3 Physico-chemical properties

Not relevant for the current proposal.

2 HARMONISED CLASSIFICATION AND LABELLING

The RAC has adopted an opinion[4] at RAC-25 that *1,2-benzenedicarboxylic acid, dihexyl ester, branched and linear* meets the following criteria for classification and labelling:

Table 2 The RAC opinion on classification and labelling in accordance with Regulation (EC) No 1272/2008 (CLP)

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-Benzene-dicarboxylic acid, dihexyl ester, branched and linear	271-093-5	68515-50-4	Repr. 1B	H360FD	GHS08 Dgr	H360FD			

Table 3 The RAC opinion on classification and labelling in accordance with Directive 67/548/EEC

Index No	Chemical Name	EC No	CAS No	Classification	Labelling	Concentration Limits	Notes
	1,2-Benzenedicarboxylic acid, dihexyl ester, branched and linear	271-093-5	68515-50-4	Repr. Cat. 2; R60-61	T R: 60-61 S: 45-53		

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

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

[4] Committee for Risk Assessment RAC Opinion proposing harmonised classification and labelling at EU level of 1,2-Benzenedicarboxylic acid, dihexylester, branched and linear EC number: 271-093-5 CAS number: 68515-50-4 CLH-O-0000002695-67-03/F Adopted 7 June 2013 http://echa.europa.eu/documents/10162/18d3ed6d-91c5-48d0-844a-8383ab5723b3

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 CMR assessment

In accordance with Article 37(4) of the CLP Regulation, the Committee for Risk Assessment (RAC) has adopted an opinion for harmonised classification and labelling of *1,2-benzenedicarboxylic acid, dihexyl ester, branched and linear* in June 2013. At RAC-25 the RAC adopted the opinion that *1,2-benzenedicarboxylic acid, dihexyl ester, branched and linear* meets the criteria for classification as toxic for reproduction Repr. 1B, H360FD ("May damage fertility. May damage the unborn child."). The corresponding classification in accordance with Directive 67/548/EEC would be toxic for reproduction Repr. Cat.2, R60-61 ("May impair fertility. May cause harm to the unborn child."). After decision of the European Commission, confirming the classification as Repr. 1B, the new classification will be included in the list of harmonised classifications (Annex VI to the CLP Regulation).

Therefore, *1,2-benzenedicarboxylic acid, dihexyl ester, branched and linear* meets the criteria of Article 57(c) of Regulation (EC) 1907/2006 (REACH Regulation).

PART II

INFORMATION ON USE, EXPOSURE, ALTERNATIVES AND RISKS

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

7.1 Information on Manufacture, Import/Export

1,2-Benzenedicarboxylic acid, dihexyl ester, branched and linear was pre-registered under REACH with indication of registration by 30 November 2010. According to recently performed searches on the ECHA website there are currently no registrations for this substance but it is possible that it could be registered at a later date.

In the Classification & Labelling Inventory there is one aggregated notification (Repr. 2, H361 Suspected of damaging fertility or the unborn child) by 14 notifiers, indicating that the substance is on the EU market (ECHA 2014).

Since there is a RAC opinion on harmonised classification of the substance that, after decision of the European Commission, will be included in Annex VI to the CLP regulation, registration is expected to follow after that inclusion if the substance is manufactured or imported to the EU in quantities of 1 tonne or more per year. However, since substances that are subject to (future) registration shall be notified to the Classification & Labelling Inventory, even if not classified, it is assumed that there is no major use of the substance by actors who until now have regarded the substance as harmless.

The substance has not been reported by EU Industry as an HPVC or LPVC according to the previous existing substances regulation (ESIS 2013).

The website Chemical Book listed 45 global suppliers for the CAS no 68515-50-4, thereof 25 in USA, 8 in China, 7 in Europe and 5 others. These figures are however uncertain, since among the synonyms listed in the “Chemical Book” for this CAS No., also the pure linear hexyl phthalate has been included (Chemical Book 2014).

7.2 Information on Uses

The SPIN database lists for 2011 that *1,2-benzenedicarboxylic acid, dihexyl ester, branched and linear* occurs in chemical mixtures on the Nordic market (Sweden, Denmark and Finland), including consumer available products. Further non-confidential information about use categories is not available in the database. The substance is reported in mixtures on the Nordic market with 1-4 tonnes per annum during the years 2002 to 2011 (excluding confidential tonnage). No further non-confidential information about tonnage and use is available (SPIN 2014).

Indications of trends in total quantities and number of preparations containing the substance can also be found in the SPIN database. Figure 1 and Figure 2 shows that the reported total amount of the substance in preparations in the Nordic countries has decreased from approximately 4 tonnes in 2006 to 1 tonne in 2011, and that the number of preparations containing the substance has been more or less

constant over the years. Figures for Finland are confidential and are not shown. Norway has not reported any products (SPIN 2014).

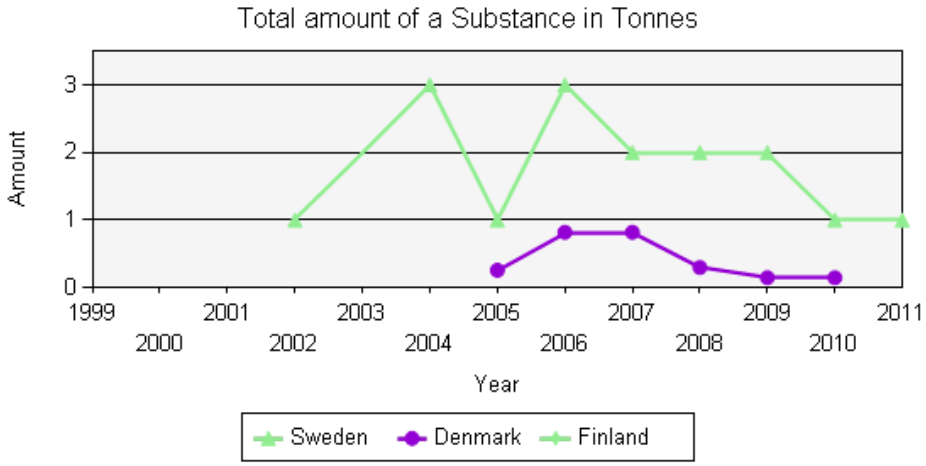


Figure 1 Total amount of the substance in preparations in Nordic countries, 1999-2011 (SPIN 2014)

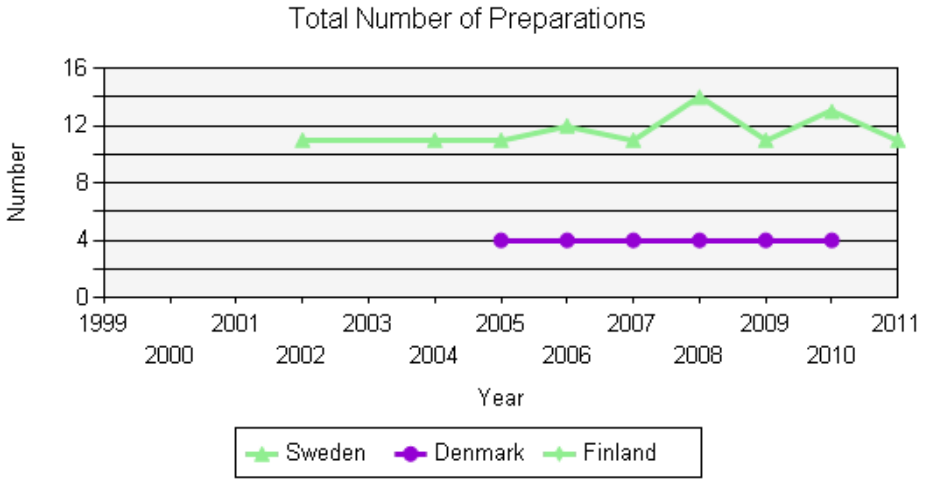


Figure 2 Total number of preparations containing the substance in Nordic countries, 1999-2011 (SPIN 2014)

The use of the substance in sealant/jointing agents (substance concentration 5-10%) on the US market (MSDS 2013) indicates that the substance can be found in imported articles. The substance has also been declared as a component in engine oil stabilizer (unknown concentration) on the US market (MSDS 2008) and in automotive gear lubricant (substance concentration 0.5 - <5%) on the German market (MSDS 2012).

The German Annex XV dossier of the structurally similar di-n-hexyl phthalate (DnHP) indicates a use as plasticiser in polymers (DE Annex XV dossier). Such use of *1,2-benzenedicarboxylic acid, dihexyl ester, branched and linear* is not found in the Swedish Products register[5] (during 1992-2012, KemI 2013). However, that use may occur in other countries or in imported articles.

[5] The Products Register does not contain information on potential presence of the substance in imported articles, but do contain information on substances in raw materials (substances and mixtures) for production of e.g. plastics.

According to Plasticisers and Flexible PVC Information Centre, low phthalates (3-6 carbon atoms in their chemical backbone), are commonly used in medical devices (DEHP), general purpose PVC (DEHP), adhesives and inks (DIBP). The most common types of low phthalates include DEHP, DBP, DIBP and BBP. They represent less than 11% of the European market. DBP, BBP and DEHP have been included on Annex XIV of the REACH regulation and will be phased out unless an application for authorisation is granted. No information on uses of the C6 phthalate *1,2-benzenedicarboxylic acid, dihexyl ester, branched and linear* can be found on the Center´s website. (Plasticisers 2014).

If technically possible, the C6 phthalate *1,2-benzenedicarboxylic acid, dihexyl ester, branched and linear* might be used as a substitute for other low/transitional phthalates of carbon backbone lengths of C4-C6 that are being phased out.

Measurements of *1,2-benzenedicarboxylic acid, dihexyl ester, branched and linear* in consumer products could indicate where the substance is used, but no such measurements are available. However, monitoring of DnHP in consumer articles are available and is relevant also for *1,2-benzenedicarboxylic acid, dihexyl ester, branched and linear* (since it is one of the substance components). DnHP was not found in a survey of different consumer products (cell phone covers, work gloves/household gloves, sleeping mats, handbags made of synthetic leather, and sneakers) (DK-EPA 2012). In another survey on textile products (swaddling clothes, bathrobe, t-shirts, pantyhose, beach dress, upholstery fabric, carpets) only small amounts (0.01 - 0.03 mg/kg) of DnHP were detected in three products (Pfordt et al. (1999)).

7.3 Information on Exposure

An initial exposure estimation based on the use pattern of *1,2-benzenedicarboxylic acid, dihexyl ester, branched and linear* has been done in the SPIN Exposure Toolbox (Nordic market in 2011, SPIN Database 2013) and it indicates a probable potential exposure of workers, consumers, and soil compartments. This is probably based on the indicated use as additives for lubricating products for motor vehicles. The information in SPIN also indicates that the range of use is in a “narrow range of applications” on the Nordic market (SPIN 2014).

The presence/absence of DnHP (which is a component of the *1,2-benzenedicarboxylic acid, dihexyl ester, branched and linear*) in house dust is an indicator for consumer exposure. Only two house dust studies of DnHP can be identified in Europe. No (Pfordt et al. 1999) and low (Watson et al. 2006) concentrations (< 4 µg/g), respectively, were detected.

After inclusion of the harmonised classification in Annex VI to the CLP regulation, the substance will be covered by Annex XVII (entry 30) to REACH and thus, in the future, shall not be placed on the market, or used, in mixtures for supply to the general public. Presence in imported articles will not be affected (unless regulated elsewhere, such as toys).

Quantification of use and exposure is not possible due to lack of data.

8 CURRENT KNOWLEDGE ON ALTERNATIVES

The information found on potential alternatives refers to the use of phthalates as plasticisers. Alternative substances could then technically be other phthalates with short or long carbon backbones, depending on the physicochemical property needed. However, one has to be aware that these may have similar reprotoxic effects as *1,2-benzenedicarboxylic acid, dihexyl ester, branched and linear* (DE Annex XV dossier 2013).

Alternatives for other low/transitional phthalates may be of interest as alternatives for *1,2-benzenedicarboxylic acid, dihexyl ester, branched and linear* too. Assesment of alternatives for DEHP,

BBP, DBP and DIBP can be found in the RAC/SEAC background document to the opinion on the Annex XV dossier proposing restrictions on those phthalates (ECHA 2012).

Regarding the use of *1,2-benzenedicarboxylic acid, dihexyl ester, branched and linear* in lubricants and additives there were 12 products containing the substance reported to the Swedish products register in 2012. In the same year there were in total 6432 products reported as lubricants and additives, i.e. 6420 products were reported without stating any content of *1,2-benzenedicarboxylic acid, dihexyl ester, branched and linear*. This may however be due to the fact that *1,2-benzenedicarboxylic acid, dihexyl ester, branched and linear* in many cases, because of how the products register regulation is written, probably was not obligatory to declare. That may also mean that more than 12 products could contain the substance (KemI 2013).

9 REFERENCES

- Chemical Book (2014). Accessed 2014-01-07. Available from: http://www.chemicalbook.com/ProdSupplierGWCB8256788_EN.htm. Accessed 2014-01-07.
- DE Annex XV dossier (2013). Proposal for identification of a substance as a CMR 1A or 1B, PBT, vPvB or a substance of an equivalent level of concern, CAS-no 84-75-3. http://echa.europa.eu/documents/10162/9a8b4fa6-c852-48bd-b561-c727b8d197ff.
- DK-EPA (2012). Nørgaard Andersen D, Møller L, Buchardt Boyd H, Boberg J, Axelstad Petersen M, Christiansen S, Hass U, Brunn Poulsen P, Strandesen M, Bach D (2012) Exposure of pregnant consumers to suspected endocrine disruptors, Survey of chemical substances in consumer products no. 117, Danish Environmental Protection Agency.
- ECHA (2012). Committee for Risk Assessment (RAC). Committee for Socio-economic Analysis (SEAC). Background document to the Opinion on the Annex XV dossier proposing restrictions on four phthalates ECHA/RAC/RES-O-0000001412-86-07/S1 ECHA/SEAC/[reference code to be added after the adoption of the SEAC opinion] http://echa.europa.eu/documents/10162/76f9edea-740c-402f-a984-1005e91a94ab.
- ECHA (2014) Classification & Labelling Inventory. Accessed 2014-01-07. http://clp-inventory.echa.europa.eu/SummaryOfClassAndLabelling.aspx?SubstanceID=28623&HarmOnly=no?fc=true&lang=en.
- ESIS (2013). European chemical Substances Information System. http://esis.jrc.ec.europa.eu/.
- KemI (2013). Advanced search in the Swedish Product Register (1992-2012). Swedish Chemicals Agency.
- MSDS (2008). Material Safety Data Sheet, Prolong Engine oil stabilizer. http://www.prolong.com/downloads/msds-2008-0630-oil%20stabilizer.pdf.
- MSDS (2012). Material Safety Data Sheet, BOT 154 LM 2, BP Europa SE. http://msdspds.bp.com/ussds/amersdsf.nsf/0/2DE3D6E30F7CCDA280257A33005453CB/$file/132671BOT%20154%20%20LM%202.pdf.
- MSDS (2013). Material Safety Data Sheet, Acrylic latex caulk. http://hdsupplysolutions.com/wcsstore/B2BDirectStorefrontAssetStore/1_Recode/product/fm/additional/MS/MSDS-108611.pdf.
- Pfordt J, Bruns-Weller E (1999). Die Phthalsäureester als eine Gruppe von Umweltchemikalien mit endokrinem Potential. Bericht über eine Auswertung der wissenschaftlichen Literatur sowie Messungen der Belastung von Lebensmitteln, Textilien und Hausstaub mit Phthalsäureestern. Niedersächsisches Ministerium für Ernährung, Landwirtschaft und Forsten (Hrsg), Verbraucherschutz, Hannover.

- Plasticisers (2014). Plasticisers and Flexible PVC Information Centre. Accessed 2014-01-09. http://www.plasticisers.org/en_GB/plasticisers/low-phthalates.
- SPIN Database (2014). Accessed 2013-11-06, 2014-01-10. http://195.215.251.229/DotNetNuke/default.aspx.
- Watson A, Eng C, Danger Dust (2006). Will REACH Protect the Public from the PBDES, Phthalates and Nonylphenols currently found in Dust and Rainwater in the Czech Republic? Arnika – Toxic and waste program, Chlumova 17, 130 00 Praha 3.