Ministry of Environment
and Water, Bulgaria

Justification Document for the Selection of a CoRAP Substance

Substance Name (public name):	**1,4-diisopropylbenzene**
EC Number:	**202-826-9**
CAS Number:	**100-18-5**
Authority:	**BG MSCA**
Date:	**22/03/2016**

Note

This document has been prepared by the evaluating Member State given in the CoRAP update.

Contents

1 IDENTITY OF THE SUBSTANCE

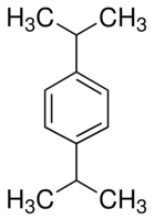
1.1 Other identifiers of the substance

Table: Other Substance identifiers

EC name (public):	**1,4-diisopropylbenzene**
IUPAC name (public):	**1,4-di(propan-2-yl)benzene**
Index number in Annex VI of the CLP Regulation:	--
Molecular formula:	**$C_{12}H_{18}$**
Molecular weight or molecular weight range:	**162.2713**
Synonyms:	**p-Diisopropylbenzene**

Type of substance ☒ Mono-constituent ☐ Multi-constituent ☐ UVCB

Structural formula:



Other relevant information about substance composition

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1.2 Similar substances/grouping possibilities

The diisopropylbenzene (DIPB) category consists of a group of three chemicals consisting of CAS No. 99-62-7, 100-18-5, and 25321-09-9. The two first members of the category , meta-DIPB (99-62-7) and para-DIPB (100-18-5), are pure isomers while the third member (xDIPB) is a Class II chemical consisting of a mixture of all three ortho-, meta-, and para-DIPB isomers.

xDIPB may contain small amounts of cumene and other aromatic hydrocarbon impurities[1]. The ortho-DIPB is not registered under REACH and no information is available. The three DIPB, CAS No. 99-62-7 (meta-DIPB), 100-18-5 (para-DIPB) and 577-55-9 (ortho-DIPB) that constitute the DIPB category are obviously very similar from a structural standpoint as they are all isomers of the same compound and possess nearly identical physical-chemical properties. It has been considered

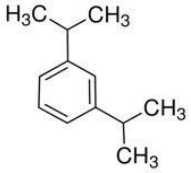
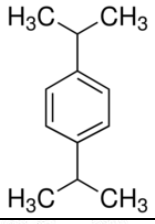
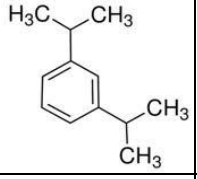
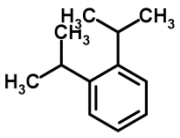
[1] HPV challenge program, diisopropylbenzene (DIPB) category, test plan, October 3, 2002.

within the HPV Program assessment that data from studies conducted on the mixture itself (xDIPB) and each of the individual isomers could be used interchangeably in the evaluation of their environmental fate, ecotoxicity, and mammalian toxicity potentials. The impurities reported in the composition of xDIPB are not taken into account in the frame of the manual screening but may be relevant for further assessment.

The substance diisopropylbenzene (xDIPB), consisiting of three chemicals with CAS No. 99-62-7 (meta-DIPB), 100-18-5 (para-DIPB) and 577-55-9 (ortho-DIPB) was manually screened by France on 27 May 2014 and is included in CoRAP 2015-2017 for SEV in 2017.

The registered substance 1,4-diisopropylbenzene (para-DIPB, CAS No. 100-18-5) is the substance of interest for this justification document and is structurally similar to 1,3-diisopropylbenzene (meta-DIPB, CAS No. 99-62-7) and diisopropylbenzene (xDIPB) mixture (CAS No. 25321-09-9).

Table 1: Similar substances, category approach

EC name	EC and CAS numbers	Structural formula	Molecular formula	Molecular weight
Diisopropylbenzene (xDIBP, mixture of par-, ortho- and meta-DIBP)	EC: 246-835-6 CAS: 25321-09-9		$C_{12}H_{18}$	162,27
1,4-diisopropylbenzene (para-DIBP)	EC: 202-826-9 CAS: 100-18-5		$C_{12}H_{18}$	162,27
1,3-diisopropylbenzene (meta-DIBP)	EC: 202-773-1 CAS: 99-62-7		$C_{12}H_{18}$	162,27
1,2-bis(1-methylethyl)benzene (ortho-DIPB)	EC: 209-412-7 CAS: 577-55-9		$C_{12}H_{18}$	162,27

2 OVERVIEW OF OTHER PROCESSES / EU LEGISLATION

Table: Completed or ongoing processes

RMOA	☐ Risk Management Option Analysis (RMOA)	
REACH Processes	Evaluation	☐ Compliance check, Final decision
		☒ Testing proposal
		☐ CoRAP and Substance Evaluation
	Authorisation	☐ Candidate List
		☐ Annex XIV
	Restri -ction	☐ Annex XVII[2]
Harmonised C&L	☐ Annex VI (CLP) (see section 3.1)	
Processes under other EU legislation	☐ Plant Protection Products Regulation Regulation (EC) No 1107/2009	
	☐ Biocidal Product Regulation Regulation (EU) 528/2012 and amendments	
Previous legislation	☐ Dangerous substances Directive Directive 67/548/EEC (NONS)	
	☐ Existing Substances Regulation Regulation 793/93/EEC (RAR/RRS)	
(UNEP) Stockholm convention (POPs Protocol)	☐ Assessment	
	☐ In relevant Annex	

[2] Please specify the relevant entry.

Other processes / EU legislation	☐ Other (provide further details below)

Ongoing Testing proposals: under Evaluation based on the registration dossier as submitted (dossier updated on 03 August 2015).

1. Sub-chronic toxicity (90-day) study: oral route (OECD 408: Repeated Dose 90-Day Oral Toxicity in Rodents), testing proposed with CAS no. 99-62-7. Deadline for submitting information: the study to be conducted in due course following approval by ECHA.
2. Combined Repeated dose toxicity study:oral route (OECD 422: Combined Repeated Dose Toxicity Study with the Reproduction / Developmental Toxicity Screening Test), testing proposed with CAS no. 100-18-5. Deadline for submitting information: the study will begin August-September 2015, and a final report will be available by 1st quarter 2016.
3. Reproductive toxicity (prenatal developmental toxicity) study (OECD 414: Prenatal Developmental Toxicity Study), testing proposed with CAS no. 99-62-7. Deadline for submitting information: the study to be conducted in due course following approval by ECHA.

Source: ECHA WEB site, 05/10/2015.

3 HAZARD INFORMATION (INCLUDING CLASSIFICATION)

3.1 Classification

3.1.1 Harmonised Classification in Annex VI of the CLP

There is no harmonised classification of the substance under Annex VI of the CLP.

3.1.2 Self classification

- In the registration:

Registrant self-classifies the substance as:

Skin Irrit. 2, H315 Causes skin irritation.

- The following hazard classes are in addition notified among the aggregated self classifications in the C&L Inventory:

Acute Tox. 4, H302: Harmful if swallowed.
Acute Tox. 4, H312: Harmful in contact with skin.
Skin Irrit. 2, H315 Causes skin irritation.
Eye Irrit. 2 H319: Causes serious eye irritation.
Acute Tox. 4, H332: Harmful if inhaled.
STOT SE 3, H335: May cause respiratory irritation.
Repr. 2, H361: Suspected of damaging fertility or the unborn child.
Aquatic Acute 1, H400: Very toxic to aquatic life
Aquatic Chronic 1, H410: Very toxic to aquatic life with long lasting effects.
Aquatic Chronic 4, H413: May cause long lasting harmful effects to aquatic life.

3.1.3 Proposal for Harmonised Classification in Annex VI of the CLP

No harmonized classification is proposed for this substance.

4 INFORMATION ON (AGGREGATED) TONNAGE AND USES[3]

4.1 Tonnage and registration status

Table: Tonnage and registration status

From ECHA dissemination site		
☒ Full registration(s) (Art. 10)	☐ Intermediate registration(s) (Art. 17 and/or 18)	
Tonnage band (as per dissemination site)		
☐ 1 – 10 tpa	☒ 10 – 100 tpa	☐ 100 – 1000 tpa
☐ 1000 – 10,000 tpa	☐ 10,000 – 100,000 tpa	☐ 100,000 – 1,000,000 tpa
☐ 1,000,000 – 10,000,000 tpa	☐ 10,000,000 – 100,000,000 tpa	☐ > 100,000,000 tpa
☐ <1 . . . . . >+ tpa (e.g. 10+ ; 100+ ; 10,000+ tpa)		☐ Confidential
Joint Submission.		

4.2 Overview of uses

Table: UsesPart 1:

☒ Manufacture	☒ Formulation	☒ Industrial use	☒ Professional use	☐ Consumer use	☐ Article service life	☒ Closed system
The identified uses of the substance are: <u>Uses at industrial sites</u>: • Industrial uses as Process Solvent for Print Inks • Use as an Intermediate <u>Uses by Professional Workers:</u> Professional Laboratory Use						

[3] *Please provide here the date when the dissemination site was accessed.*

5. JUSTIFICATION FOR THE SELECTION OF THE CANDIDATE CoRAP SUBSTANCE

5.1. Legal basis for the proposal

☒ Article 44(2) (refined prioritisation criteria for substance evaluation)

☐ Article 45(5) (Member State priority)

5.2. Selection criteria met (why the substance qualifies for being in CoRAP)

☒ Fulfils criteria as CMR/ Suspected CMR

☐ Fulfils criteria as Sensitiser/ Suspected sensitiser

☐ Fulfils criteria as potential endocrine disrupter

☒ Fulfils criteria as PBT/vPvB / Suspected PBT/vPvB

☐ Fulfils criteria high (aggregated) tonnage (*tpa > 1000*)

☒ Fulfils exposure criteria

☐ Fulfils MS's (national) priorities

5.3 Initial grounds for concern to be clarified under Substance Evaluation

Hazard based concerns		
CMR ☐ C ☐ M ☐ R	Suspected CMR ☐ C ☐ M ☒ R	☐ Potential endocrine disruptor
☐ Sensitiser	☐ Suspected Sensitiser	
☐ PBT/vPvB	☒ Suspected PBT/vPvB[1]	☐ Other (please specify below)

Exposure/risk based concerns		
☐ Wi☐e dispersive use	☐ Consumer use	☐ Exposure of sensitive populations
☐ Exposure of environment	☒ Exposure of workers	☐ Cumulative exposure
☐ High RCR	☐ High (aggregated) tonnage	☐ Other (please specify below)

Regarding the suspected PBT/vPvB concern

The registered substance is not readily degradable according to the available data in the dossier. However, the biodegradation data are considered insufficient and not fully satisfactory to assess P/vP properties. The registrant stated that no conclusion can be reached based on available information; however no indication of a testing proposal is provided in the dossier. Based on estimated and experimental data, the substance fulfils the screening criteria for P and leaves the potential for vP. There is a lack of data to fully assess P or vP. Further assessment is considered needed on the P/vP criterion.

Based on the provided experimental Log Kow of 5.23, the substance fulfils the B criterion on screening. The substance is considered stable in the aquatic compartment. Based on a provided read-across bioaccumulation study, the B criterion is clearly fulfilled (with BCF>2000<5000) on screening. No bioaccumulation, biota-sediment accumulation, and biomagnification factors (BAF, BSAF, BMF) are provided in the registration dossier. Based on the bioaccumulation estimated data for BCF, the substace indicate a potential for vB (>5000). Therefore, the substance clearly fulfills the B criterion and is potentially vB on screening based on experimental and estimated data. Further assessment is considered needed on the B/vB criterion.

The substance is presented by the registrant to not fulfill the T criterion, but further information is necessary to conclude on the T properties in the context of the PBT assessment. Based on the estimated chronic aquatic toxicity data, the substance is to be considered as fulfilling the T criterion on screening. Depending on the P/vP and B/vB outcome, the aquatic chronic toxicity could be further investigated. Moreover the notifications of classification as aquatic chronic 1 (H410) should be further assessed.

Regarding the Suspected Reproductive Toxicity concern

If the substance is included in the CoRAP list because of its PBT properties, the proposed studies should be evaluated in order to clarify the concern associated with the notified Repr. 2 classification. In addition, if reproductive toxicity is verified, workplace exposure scenarios and risk characterization taking into account Council Directive 92/85/EEC and Directive 98/24/EC („Chemical Agents Directive") would be needed.

Conclusion:

The substance to be included in the CoRAP 2016-2018 list for evaluation in 2018.

References:

1. EPIWEB 4.1 (US EPA, Nov. 2012). Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11 or insert version used]. United States Environmental Protection Agency, Washington, DC, USA.
2. PBT profiler (http://www.pbtprofiler.net/): Developed by the Environmental Health Analysis Center under contract to the Office of Chemical Safety and Pollution Prevention , U.S. Environmental Protection Agency Computer Resources Donated by SRC, Inc. Ver 2.000 Last Updated September 4, 2012.
3. ECOSAR™ estimation program (http://www.pbtprofiler.net/ecosarres.asp?I=0&K=4.905), ECOSAR Version 1.11.
4. www.echemportal.org, OECD SIDS INITIAL ASSESSMENT PROFILE of 1,4-diisopropylbenzene.
5. http://webnet.oecd.org/CCRWEB/ChemicalDetails.aspx?Key=567a7cdf-4925-4ae3-90da-c8c35a211a30&Idx=0

5.4 Preliminary indication of information that may need to be requested to clarify the concern

☒ Information on toxicological properties	☐ Information on physico-chemical properties
☒ Infomation on fate and behaviour	☒ Information on exposure
☒Information on ecotoxicological properties	☐ Information on uses
☐ Information ED potential	☐ Other (provide further details below)

Suspected PBT or vP/VB concern

Additional information is required to conclude on PBT or vP/vB properties.

Depending on the P/vP and B/vB outcome, the aquatic chronic toxicity (on other species than aquatic invertebrates) might need to be investigated further to conclude on the T properties in the context of the PBT assessment.

Suspected Reproductive Toxicity concern

If the substance is included in the CoRAP list because of its PBT properties, the proposed studies should be evaluated in order to clarify the concern associated with the notified Repr. 2 classification. In addition, if reproductive toxicity is verified, workplace exposure scenarios and risk characterization taking into account Council Directive 92/85/EEC and Directive 98/24/EC („Chemical Agents Directive") should be needed.

Conclusion:

The substance to be included in the CoRAP 2016-2018 list for evaluation for 2018.

5.5 Potential follow-up and link to risk management

☐Harmonised C&L	☒ Restriction	☒ Authorisation	☐ Other (provide further details)

If the substance is identified/evaluated as a PBT/vPvB substance, an analysis of risk management options (RMOA) will be carried out, taking into account information on use and exposure. Potential options are the inclusion in the Candidate List with or without Authorisation, but also Restriction.