Ministry of Environment
and Water, Bulgaria

Justification Document for the Selection of a CoRAP Substance

Substance Name (public name):	**1,3-diisopropylbenzene**
EC Number:	**202-773-1**
CAS Number:	**99-62-7**
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

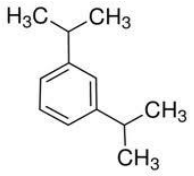
1.1 Other identifiers of the substance

Table: Substance identy

EC name (public):	**1,3-diisopropylbenzene**
IUPAC name (public):	**1,3-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:	**162.140850576**
Synonyms:	

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 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.

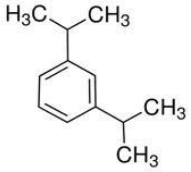
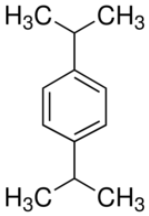
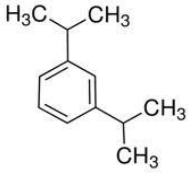
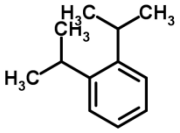
[1] HPV challenge program, diisopropylbenzene (DIPB) category, test plan, October 3, 2002.

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. The substance is included in CoRAP 2015-2017 for SEV by France in 2017.

The registered substance 1,3-diisopropylbenzene (meta-DIPB, Cas No. 99-62-7) is the substance of interest for this justification document and is structurally similar to1,4-diisopropylbenzene (para-DIPB, CAS No. 100-18-5) and diisopropylbenzene (xDIPB) mixture (CAS No. 25321-09-9).

The two impurities reported in the composition of meta-DIPB are not taken into account in the frame of the manual screening but may be relevant for further assessment.

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)
ECHA decision on testing proposal(s) set out in a registration pursuant to article 40(3) of Regulation (EC) NO 1907/2006 – Decision number: TPE-D-2114289305-44-01/F, Helsinki, 19 December 2014. Ongoing testing, required pursuant to Article 40(3): 1. Repeated Sub-Chronic toxicity study (90-day) in rats, oral route (test method 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. Prenatal Developmental toxicity study in rats or rabbits, oral route (test method 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. The decision is based on the registration dossier as submitted. The deadline for submitting the required information by the Registrant is 2 January 2017.	

3 HAZARD INFORMATION (INCLUDING CLASSIFICATION)

3.1 Classification

3.1.1 Harmonised Classification in Annex VI of the CLP

The substance is not classified under Annex VI of the CLP.

3.1.2 Self classification

- In the registration:

The substance is not classified by the registrant.

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

Skin iritt. 2	H315: Causes skin irritation
Eye Irrit. 2	H319: Causes serious eye irritation.
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

3.1.3 Proposal for Harmonised Classification in Annex VI of the CLP

No harmonised 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: Uses

Part 1:

☒ Manufacture	☒ Formulation	☒ Industrial use	☒ Professional use	☐ Consumer use	☐ Article service life	☒ Closed system
The identified uses of the substance are: <u>Uses as intermediate</u> • Formulation • Distribution and Storage <u>Uses at industrial sites</u>: • Industrial uses as Process Solvent (Industrial) • 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		
☐ Wide 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 5.13, 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

Suspected reproductive toxicity concern is based on Notified classification and labeling according to CLP criteria in the C&L Inventory.

Overall so far there are no indications of very high human health concern from this substance associated with workplase exposure. There is a notified classification as Repr. 2 in the C&L Inventory, however the studies provided with the registration dossier do not describe signs of reproductive toxicity. Two testing proposals are indicated as submitted to ECHA in the dossier: an oral 90 day study and one developmental toxicity study.

Thus, from the perspective of human health toxicity alone the substance would not be of highest priority for SEv. Nevertheless, 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 is 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=17

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

☒ Information on toxicological properties	☐ Information on physico-chemical properties
☒ Information 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") would be needed.

Conclusion:

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