Justification for the selection of a substance for CoRAP inclusion

Substance Name (Public Name):	Diisopropylbenzene
Chemical Group:	Diisopropylbenzene category
EC Number:	246-835-6
CAS Number:	25321-09-9
Submitted by:	FRANCE
Date:	17/03/2015

Note

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

Contents

1 IDENTITY OF THE SUBSTANCE

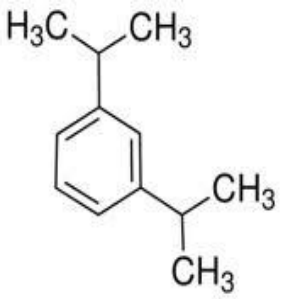
1.1 Other identifiers of the substance

Table 1: Substance identity

EC name:	Diisopropylbenzene
IUPAC name:	Di(propan-2-yl)benzene
Index number in Annex VI of the CLP Regulation	none
Molecular formula:	$C_{12}H_{18}$
Molecular weight or molecular weight range:	162.27
Synonyms/Trade names:	Benzene, bis (1-methylethyl)- Diisopropylbenzene (mixture) Diisopropylbenzene, all isomers

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

Structural formula:



1.2 Similar substances/grouping possibilities

The diisopropylbenzene (DIPB) category consists of a group of three chemicals consisting of CAS Registry Numbers 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 is the substance of interest for this justification document.

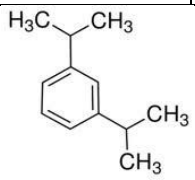
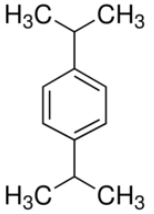
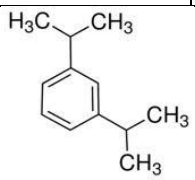
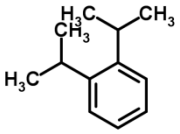
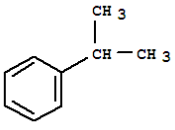
xDIPB may contain small amounts of cumene and other aromatic hydrocarbon impurities[1]. The ortho-DIPB is not registered under REACH and no information is available. The three DIPB CAS numbers that constitute the DIPB category are obviously very similar from a structural standpoint as they are all isomers of the

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

same compound and possess nearly identical physical-chemical properties; it is 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.

Since diisopropylbenzene (xDIPB) is a mixture of the 3 isomers, its assessment covers the whole category. 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. In the HPV challenge program testing plan[1], cumen is also included in the matrix of DIBP assessment.

Table 2: 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: 246-835-9 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
Isopropylbenzene (cumene)	EC: 202-704-5 CAS: 98-82-8		C_9H_{12}	

2 CLASSIFICATION AND LABELLING

2.1 Harmonised Classification in Annex VI of the CLP

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

2.2 Self classification

- In the registration

  Not classified by the registrant(s)

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

Asp. Tox. 1	H304
Eye Irrit. 2	H319
Skin Irrit. 2	H315
STOT SE 3 (inhalation)	H336 & H335
STOT RE 2 (gavage)	H373
Aquatic Acute 1	H400
Aquatic Chronic 1	H410
Aquatic Chronic 2	H411
Aquatic Chronic 4	H413

2.3 Proposal for Harmonised Classification in Annex VI of the CLP

No harmonized classification is proposed for this substance

3 INFORMATION ON AGGREGATED TONNAGE AND USES

From ECHA 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

☒ Industrial use	☐ Professional use	☐ Consumer use	☐ Closed System

At industrial sites, xDIPB is used as

- industrial intermediates in the synthesis of other chemicals for the formulation of preparations (polymer preparations and compounds),
- as solvent for gas extraction for instance for the production of organic peroxide (industrial use of substances in closed systems),
- polymerisation initiator, cross-linking agent (polymer preparations and compounds).

xDIPB is also indirectly used by professionals and consumers through the use of fertilizer additives but there is no clear indication in the dossier on potential release to the environment and/or contact during handlings.

4 OTHER COMPLETED/ONGOING REGULATORY PROCESSES THAT MAY AFFECT SUITABILITY FOR SUBSTANCE EVALUATION

☐ Compliance check, Final decision	☐ Dangerous substances Directive 67/548/EEC
☐ Testing proposal	☐ Existing Substances Regulation 793/93/EEC
☐ Annex VI (CLP)	☐ Plant Protection Products Regulation 91/414/EEC
☐ Annex XV (SVHC)	☐ Biocidal Products Directive 98/8/EEC ; Biocidal Product Regulation (Regulation (EU) 528/2012)
☐ Annex XIV (Authorisation)	☐ Other (provide further details below)
☐ Annex XVII (Restriction)	

none

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[1] ☐C ☐M ☒R	☐ Potential endocrine disruptor
☐ Sensitiser	☐ Suspected Sensitiser[2]	
☐ 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)

[2] CMR/Sensitiser: known carcinogenic and/or mutagenic and/or reprotoxic properties/known sensitising properties (according to CLP harmonized or registrant self-classification or CLP Inventory)
Suspected CMR/Suspected sensitiser: suspected carcinogenic and/or mutagenic and/or reprotoxic properties/suspected sensitising properties (not classified according to CLP harmonized or registrant self-classification)
Suspected PBT: Potentially Persistent, Bioaccumulative and Toxic

Regarding the suspected PBT/vPvB concern

Based on the provided Log Kow of both isomers, the substance fulfills the B criterion on screening. Based on a provided bioaccumulation study carried out in the frame of the HPV Challenge Program and the "Screening Information Data Set" (SIDS) OECD program, the B criterion would be fulfilled (maximum ranges of the BCF are over 2000 for both isomers). Biological factors such as growth and fish lipid content may not have been taken into consideration, leading to potential higher BCF. Further assessment is considered needed on the B/vB criterion.

The substance is considered stable in the aquatic compartment. Based on the provided biodegradation study (0% biodegradation after 14 days), the P criterion is considered to be fulfilled on screening and the substance is potentially vP. The registrant(s) state in the dossier that no conclusion can be reached and that a simulation study is needed; however no indication of a testing proposal is provided in the dossier. Further assessment is considered needed on the P/vP criterion.

The substance is presented by the registrant(s) to not fulfill the T criterion, but an in-depth assessment of the provided aquatic acute toxicity studies would be needed considering its low solubility. Depending on the P and B outcome, the aquatic chronic toxicity could be investigated. Moreover the notifications of classification as aquatic chronic 1 and 2 should be further assessed.

Regarding the suspected reproductive toxicity concern

Effects reported in the repeated doses studies and developmental effects raise a human health concern that should be further investigated.

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

ENV concern

The bioaccumulation studies should be revised in order to get a reliable estimation of bioaccumulation criteria.

In parallel, a simulation study with indication on degradation products is considered needed to conclude on the P/vP criterion.

The chronic toxicity (on other species than aquatic invertebrates) could be investigated later-on based on the P and B outcome. Considering the potential release to the soil compartment from the provided uses (see the "other" endpoint below), the terrestrial toxicity could also be envisaged beyond the already provided study on terrestrial plants that is considered not reliable.

HH concern

The substance should be considered as irritant. However, the provided data on this endpoint in the dossier are not fully satisfactory. More data would be needed to confirm this expected classification.

Some effects are seen in the repeated doses studies, some are considered as not relevant by the registrant(s) but the non relevancy is not sufficiently justified. The STOT RE property should be further investigated.

Some developmental effects are indicated in the provided studies but not yet considered by the registrant, occurring at levels with maternal toxicity. The provided conclusions and explanations are not fully satisfactory.

Other

Additionally, clarifications on end-uses and expected properties/function of the substance (use in fertilizers additives) are needed in order to assess the potential of release to the environment (especially the soil compartment) and the potential exposure of professionals and consumers of such possibly DIBP containing fertilizers.

5.5 Potential follow-up and link to risk management

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