SUBSTANCE EVALUATION CONCLUSION

as required by REACH Article 48

and

EVALUATION REPORT

for

Benzene, mono-C10-13-alkyl derives., distillation residues

EC No 284-660-7

CAS RN 84961-70-6

Evaluating Member State: Italy

Dated: 14 January 2022

Evaluating Member State Competent Authority

MSCA Italy National Institute of Health on behalf of Ministry of Health
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Year of evaluation in CoRAP: 2014

Before concluding the substance evaluation a Decision to request further information was issued on: 13 June 2016.

Further information on registered substances here:

http://echa.europa.eu/web/guest/information-on-chemicals/registered-substances

DISCLAIMER

This document has been prepared by the evaluating Member State as a part of the substance evaluation process under the REACH Regulation (EC) No 1907/2006. The information and views set out in this document are those of the author and do not necessarily reflect the position or opinion of the European Chemicals Agency or other Member States. The Agency does not guarantee the accuracy of the information included in the document. Neither the Agency nor the evaluating Member State nor any person acting on either of their behalves may be held liable for the use which may be made of the information contained therein. Statements made or information contained in the document are without prejudice to any further regulatory work that the Agency or Member States may initiate at a later stage.

Foreword

Substance evaluation is an evaluation process under REACH Regulation (EC) No. 1907/2006. Under this process the Member States perform the evaluation and ECHA secretariat coordinates the work. The Community rolling action plan (CoRAP) of substances subject to evaluation, is updated and published annually on the ECHA web site[1].

Substance evaluation is a concern driven process, which aims to clarify whether a substance constitutes a risk to human health or the environment. Member States evaluate assigned substances in the CoRAP with the objective to clarify the potential concern and, if necessary, to request further information from the registrant(s) concerning the substance. If the evaluating Member State concludes that no further information needs to be requested, the substance evaluation is completed. If additional information is required, this is sought by the evaluating Member State. The evaluating Member State then draws conclusions on how to use the existing and obtained information for the safe use of the substance.

This Conclusion document, as required by Article 48 of the REACH Regulation, provides the final outcome of the Substance Evaluation carried out by the evaluating Member State. The document consists of two parts i.e. A) the conclusion and B) the evaluation report. In the conclusion part A, the evaluating Member State considers how the information on the substance can be used for the purposes of regulatory risk management such as identification of substances of very high concern (SVHC), restriction and/or classification and labelling. In the evaluation report part B the document provides explanation how the evaluating Member State assessed and drew the conclusions from the information available.

With this Conclusion document the substance evaluation process is finished and the Commission, the Registrant(s) of the substance and the Competent Authorities of the other Member States are informed of the considerations of the evaluating Member State. In case the evaluating Member State proposes further regulatory risk management measures, this document shall not be considered initiating those other measures or processes. Further analyses may need to be performed which may change the proposed regulatory measures in this document. Since this document only reflects the views of the evaluating Member State, it does not preclude other Member States or the European Commission from initiating regulatory risk management measures which they deem appropriate.

[1] http://echa.europa.eu/regulations/reach/evaluation/substance-evaluation/community-rolling-action-plan

Contents

Part A. Conclusion

1. CONCERN(S) SUBJECT TO EVALUATION

The Substance, Benzene, mono-C10-13-alkyl derives., distillation residues (EC number 284-660-7; HAB) was originally selected for substance evaluation in order to clarify concerns about:

- Environment/suspected PBT
- Exposure/wide dispersive use
- Consumer use
- Aggregated tonnage

During the evaluation an additional concern was identified:

- Potential risk for soil compartment

2. OVERVIEW OF OTHER PROCESSES / EU LEGISLATION

Compliance Check decision (Decision number: CCH-D-0000003430-86-03/F). Information available on the ECHA dossier-evaluation-status page.

3. CONCLUSION OF SUBSTANCE EVALUATION

The evaluation of the available information on the substance has led the evaluating Member State to the following conclusions, as summarised in the table below.

Table 1

CONCLUSION OF SUBSTANCE EVALUATION	
Conclusions	**Tick box**
Need for follow-up regulatory action at EU level	
Harmonised Classification and Labelling	
Identification as SVHC (authorisation)	
Restrictions	
Other EU-wide measures	
No need for regulatory follow-up action at EU level	X

4. FOLLOW-UP AT EU LEVEL

4.1. Need for follow-up regulatory action at EU level

Not applicable.

5. CURRENTLY NO FOLLOW-UP FORESEEN AT EU LEVEL

5.1. No need for regulatory follow-up at EU level

Suspected PBT/vPvB

Based on evaluation of the biodegradation simulation studies in soil, conducted on a specific surrogate substance, 1,4-di-(2-decanyl)benzene, considered to be representative of dialkyl

benzenes, the eMSCA concludes that the Substance fulfils the P and vP criteria of Annex XIII.

The high hydrophobicity of the substances raises a concern for slow bioaccumulation which cannot be investigated further with existing validated methods. Based on the current PBT guidance (ECHA 2017) and the available data for 1,1'-(isopropylidene)bis[3,5-dibromo-4-(2,3-dibromopropoxy)benzene] (TBBPA-DBPE, EC number 244-617-5), the eMSCA concludes that the B criterion of Annex XIII is likely not fulfilled.

Based on the currently available information, the eMSCA concludes that the substance is not considered to fulfil the T criterion of Annex XIII.

Potential risk for soil compartment

Newly submitted data provide sufficient and reliable evidence of no concern for terrestrial organisms. No further action is needed.

For all uses, the risk management measures and operational conditions, are appropriate and the risk is adequately controlled in all the environmental compartments.

The exposure for workers has been correctly addressed including the identification of the appropriate Risk Management Measures. For human health both exposure and risk assessment has been properly carried out and no potential risk for consumers has been highlighted.

Table 2

REASON FOR REMOVED CONCERN The concern could be removed because	Tick box
Clarification of hazard properties/exposure	X
Actions by the registrants to ensure safety, as reflected in the registration dossiers (e.g. change in supported uses, applied risk management measures, etc.)	

5.2. Other actions

Not Applicable.

6. TENTATIVE PLAN FOR FOLLOW-UP ACTIONS (IF NECESSARY)

Not Applicable.

Part B. Substance evaluation

7. EVALUATION REPORT

The Substance evaluation has started on April 2014.

7.1. Overview of the substance evaluation performed

The Substance, Benzene, mono-C10-13-alkyl derives., distillation residues (EC number 284-660-7; HAB) was originally selected for substance evaluation in order to clarify concerns about:

- Environment/suspected PBT
- Exposure/wide dispersive use
- Consumer use
- Aggregated tonnage

During the evaluation an additional concern was identified:

- Potential risk for soil compartment

Table 3

EVALUATED ENDPOINTS	
Endpoint evaluated	**Outcome / conclusion**
Suspected PBT/vPvB	Concern refuted P/vP confirmed: Based on evaluation of the biodegradation simulation studies in soil, conducted on a specific surrogate substance, 1,4-di-(2-decanyl)benzene, considered representative of dialkyl benzenes, it can be concluded that the substance fulfills the P and vP criteria of Annex XIII. B/vB unresolved: The high hydrophobicity of the substances (logKow > 10) raises a concern for slow bioaccumulation which cannot be investigated further with existing validated methods. Based on the currently available PBT guidance (ECHA 2017) and the available data for TBBPA-DBPE, the eMSCA concludes that the B criterion is likely not fulfilled. T refuted: Substance does not meet the T criteria based on human health classification and is not classified according to CLP. Available aquatic toxicity data show that the substance is generally considered non-toxic to aquatic organisms within the limits of water solubility. Consequently, the substance is not considered to fulfil the T criterion.
Potential risk for soil compartment	Concern refuted Request fulfilled by the Registrant(s). Newly submitted data provide sufficient and reliable evidence of no concern for terrestrial organisms . No further action is needed.
Exposure/wide dispersive use	The exposure for workers has been correctly addressed including the identification of the appropriate Risk Management Measures.
Consumer use	Concern refuted For human health both exposure and risk assessment has been properly carried out and no potential risk for consumers has been highlighted.

Environmental exposure assessment and risk characterisation	Concern refuted Request fulfilled by the Registrant(s). For all uses, the risk management measures and operational conditions, are appropriate and the risk is adequately controlled in all the environmental compartments.

7.2. Procedure

The Substance evaluation was started on April 2014.
In the course of the evaluation, the evaluating MSCA identified additional concerns regarding potential risk for soil compartment. Therefore, it prepared a draft decision pursuant to Article 46(1) of REACH to request further information. It submitted the draft decision to ECHA on 26 March 2015.

A unanimous agreement of the Member State Committee on the draft decision was reached on 12 April 2016 in a written procedure launched on 1 April 2016.

ECHA took the decision pursuant to Article 51(6) of REACH, requesting further information to clarify the concern for PBT/vPvB.

Subsequently the Registrant(s) updated the dossier with the requested information. Following the assessment, the eMSCA concluded that no further action is needed.

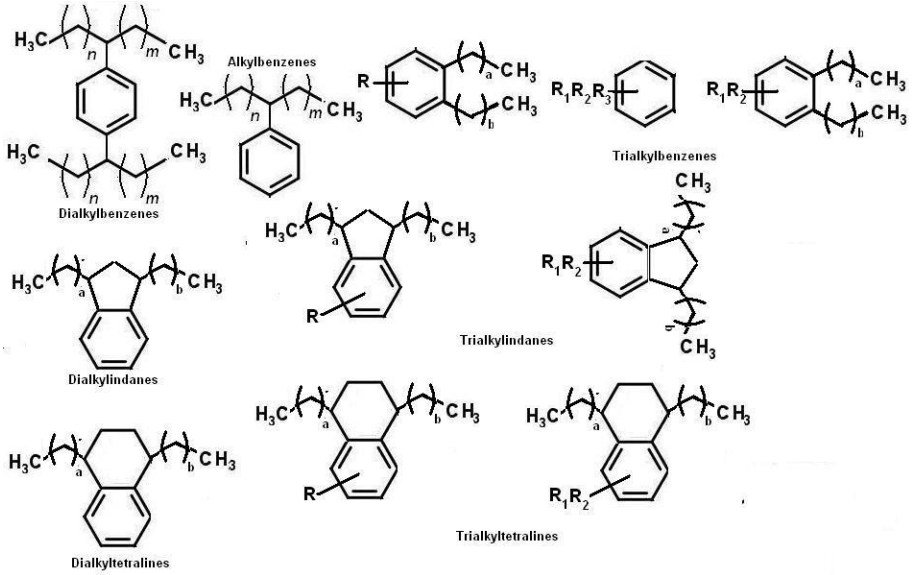
7.3. Identity of the substance

Table 4

SUBSTANCE IDENTITY	
Public name:	Benzene, mono-C10-13-alkyl derivs., distn. residues
EC number:	284-660-7
CAS number:	84961-70-6
Index number in Annex VI of the CLP Regulation:	--
Molecular formula:	Not available - not a single isomer
Molecular weight range:	--
Synonyms:	C10-13 HAB 81691-70-6; HAB

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

Structural formula:



Multiconstituent / UVCB substance / others

The Substance HAB is an extremely complex hydrocarbon UVCB.

The Substance is comprised of 21 different categories of components.

The total number of individual components is estimated to be nearly 1000. The categories are: 1) dialkyl benzenes, 2) trialkyl benzenes, 3) alkyl dialkyl benzenes, 4) monoalkyl benzenes, 5) alkylindanes, 6)Alkyl Tetra-hydronaphthalenes, 7) Alkyl Alkylene Benzenes, 8) Alkyl Octahydroanthracenes, 9)Alkylindenes, 10) Alkyl Dialkyl Dihydronaphthalenes, 11) Alkyl Tetraalkyl Dihydronaphthalenes, 12) Alkyl Alkylene Dihydronaphthalenes, 13) Alkylnaphthalenes, 14) Diphenyl Alkanes, 15) Alkyl Diphenyl Alkanes, 16) AlkylAcenaphthenes, 17) Phenyl Alkyl Tetra-hydronaphthalenes, 18) Phenyl Alkyl Indanes, 19) Alkyl Phenyl Alkylene Benzenes, 20) Alkyl Acenaphthylenes and 21) Alkyl Fluorenes.

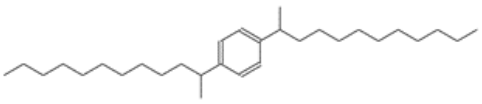
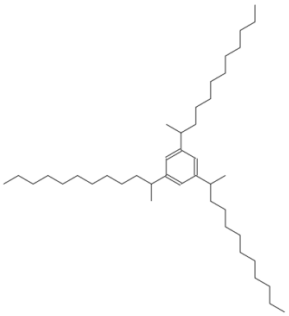
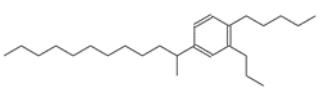
Table 5

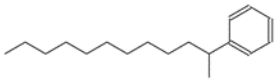
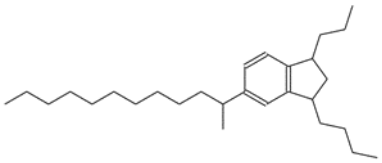
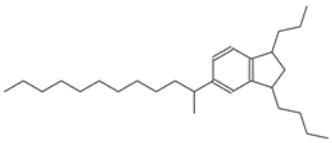
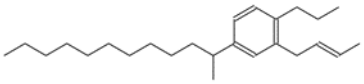
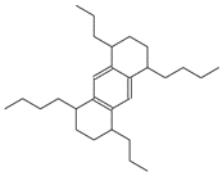
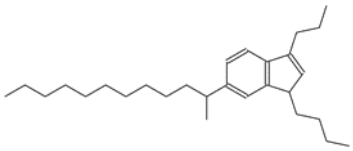
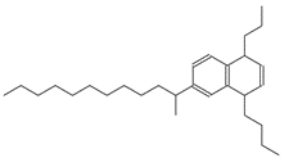
Constituents	Remarks
Legal entity composition of the substance (ECHA dissemination web)	No public concentration ranges are available for the constituents below
di-(C10-13)-benzene alkyl derivs. CnH2n-6	
Mono and di-Alkyl-(C10-13)-di-alkyl benzenes CnH2n-6	
tri-(C10-13)-benzene alkyl derivs. CnH2n-6	
Benzene, C10-13-alkyl derivs. EC Number: 267-051-0. CAS RN: 67774-74-7	
Alkyl-(C10-13)-dialkylindanes + Alkyl-(C10-13)-dialkyltetrahydronaphthalenes CnH2n-8	
Alkylalkenylbenzenes CnH2n-8	
Alkyltetraalkyldihydronaphthalene CnH2n-10	
Alkylalkenyldihydronaphthalene CnH2n-12	
Diphenylalkanes and Polylakyl diphenylalkanes CnH2n-14	
Alkylacenaphthalene CnH2n-14	

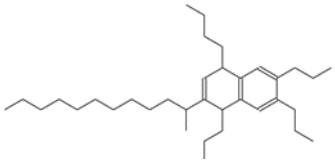
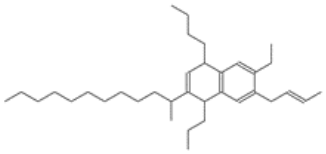
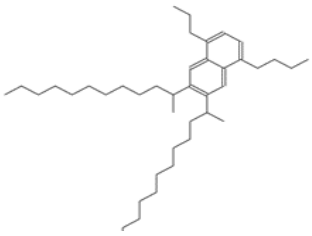
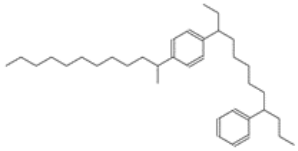
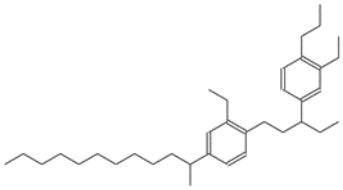
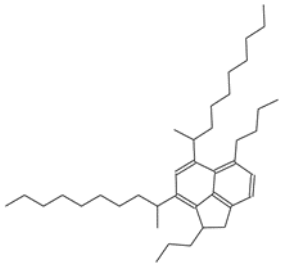
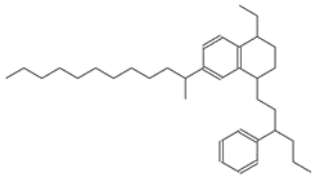
Alkylfluorene CnH2n-16	
Unknown constituents	
Benzo[def]chrysene CAS RN:50-32-8	
Fluoranthene CAS RN:206-44-0	
Pyrene CAS RN:129-00-0	
Benz[a]anthracene CAS RN:56-55-3	
Chrysene CAS RN:218-01-9	
Benzo[e]acephenanthrylene CAS RN:205-99-2	
Benzo[k]fluoranthene CAS RN:207-08-9	
Benzo[ghi]perylene CAS RN:191-24-2	
Dibenz[a,h]anthracene CAS RN : 53-70-3	
Fluorene CAS RN: 86-73-7	
Indeno[1,2,3-cd]pyrene CAS RN: 193-39-5	

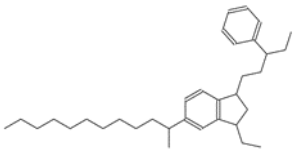
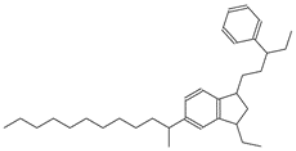
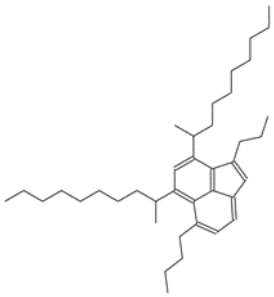
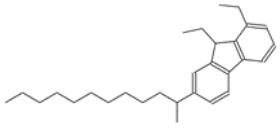
In the table below the structural formula of Representative substances used as Test material in QSAR models for each Category/Fraction are reported (ChemSpider and SMILES_generator web tools used by eMSCA).

Table 6 Representative substances of each category

Fraction	Category Representatives used for the BCF predictions (structural formula, SMILE notations and Molecular Weights)	Logk_{ow} Calc (EPIWEB 4.1)
1) dialkyl benzenes	 MW: 414.77 c1c(C(C)CCCCCCCCC)ccc(C(CCCCCCCCC)C)c1	13.74
2) trialkyl benzenes	 MW: 583.09 c1(C(C)CCCCCCCCC)cc(C(CCCCCCCCC)C)cc(C(CCCCCCCCC)C)c1	19.62
3) alkyl dialkyl benzenes	 MW: 358.66	11.91

	c1(C(C)CCCCCCCCCC)cc(CCC)c(CCCCC)cc1	
4) monoalkyl benzenes	 MW: 246.44 2-PHENYLDODECANE = 2-Dodecanylbenzene= Monoalkylbenzene – LAB CAS 2719-61-1 c1(C(C)CCCCCCCCCC)ccccc1	7.87 (8.19 LogKow exp. Sherblom PM *et al.*, 1992)
5) alkylindanes	 MW: 384.69 C1C(CCC)c2c(cc(C(C)CCCCCCCCCC)cc2)C1(CCCC)	12.63
6) Alkyl Tetra-hydronaphthalenes	 MW: 384.69 C1C(CCC)c2c(cc(C(C)CCCCCCCCCC)cc2)C1(CCCC)	12.63
7) Alkyl Alkylene Benzenes	 MW: 342.61 c1(C(C)CCCCCCCCCC)cc(CC=CC)c(CCC)cc1	11.20
8) Alkyl Octahydroanthracenes	 MW: 382.68 c32c(C(CCCC)CCC3CCC)cc1c(C(CCCC)CCC1CCC)c2	12.5
9) Alkylindenes	 MW: 382.68 C1=C(CCC)c2c(cc(C(C)CCCCCCCCCC)cc2)C1(CCCC)	12.54
10) Alkyl Dialkyl Dihydronaphthalenes	 MW: 396.71 C1=CC(CCC)c2c(cc(C(C)CCCCCCCCCC)cc2)C1(CCCC)	12.91

11) Alkyl Tetraalkyl Dihydronaphthalenes	 MW: 480.87 C1=C(C(C)CCCCCCCCCC)C(CCC)c2c(cc(CCC)c(CCC)c2)C1(CCCC)	15.97
12) Alkyl Alkylene Dihydronaphthalenes	 MW: 478.85 C1=C(C(C)CCCCCCCCCC)C(CCC)c2c(cc(CC)c(CC=CC)c2)C1(CCCC)	15.75
13) Alkylnaphthalenes	 MW: 563.02 c1(C(C)CCCCCCCCCC)c(C(C)CCCCCCCCCC)cc2c(c(CCC)ccc2(CCCC))c1	18.47
14) Diphenyl Alkanes	 MW: 4 90.86 CCC(c1ccc(C(C)CCCCCCCCCC)cc1)CCCCCC(c2ccccc2)CCC	15.38
15) Alkyl Diphenyl Alkanes	 MW: 490.86 C(c1c(CC)cc(C(C)CCCCCCCCCC)cc1)CC(c2cc(CC)c(CCC)cc2)CC	15.62
16) AlkylAcenaphthenes	 MW: 532.94 c1(CCCC)c2c3c(c(C(C)CCCCCCCC)cc2C(C)CCCCCCCC)C(CCC)Cc3cc1	17.36
17) Phenyl Alkyl Tetra-hydronaphthalenes	 MW: 488.85 c12c(C(CCC(c3ccccc3)CCC)CCC1CC)cc(C(C)CCCCCCCCCC)cc2	15.25

18) Phenyl Alkyl Indanes	 MW: 460.79 c32c(C(CC)CC3CCC(c1ccccc1)CC)cc(C(C)CCCCCCCCCC)cc2	14.27
19) Alkyl Phenyl Alkylene Benzenes	 MW: 334.55 c1(CC)c(CC(C(=CCc2c(CC)cccc2)CC)CC)cccc1	10.02
20) Alkyl Acenaphthylenes	 MW: 530.93 C1(CCC)c2c3c(c(C(C)CCCCCCCC)cc2C(C)CCCCCCCC)c(CCCC)ccc3C=1	12.27
21) Alkyl Fluorenes	 MW: 390.66 c12c3c(c(CC)ccc3)C(CC)c1cc(C(C)CCCCCCCCCC)cc2	11.56

7.4. Physico-chemical properties

Table 7

OVERVIEW OF PHYSICOCHEMICAL PROPERTIES	
Property	**Value**
Physical state at 20°C and 101.3 kPa	liquid
Vapour pressure	The vapour pressure is < 5 Pa at both 20 and 50°C
Water solubility	0.001 mg/L at 20°C
Partition coefficient n-octanol/water ($logK_{ow}$)	log Pow 9.9* at 25 °C
Flammability	Data waiving
Explosive properties	Data waiving
Oxidising properties	Data waiving
Granulometry	Data waiving
Stability in organic solvents and identity of relevant degradation products	Data waiving
Dissociation constant	Data waiving

* Registrant(s) provided data from three studies using OECD 117 showing average logK_{ow} to range from 6.6-9.9. The Registration dossier specifies the actual logK_{ow} values for each study, ranging from 6.45 to 12.53:
1. OECD Guideline 117
Test material information: Benzene, mono-C10-13-alkyl derivs., distn. residues / 84961-70-6 / 284-660-7
Being a multiconstiuent substance, several peaks were observed.
The log Pow for each fraction was 6.45, 6.64, and 6.82.
2. OECD Guideline 117
Test material information: Benzene, mono-C10-13-alkyl derivs., distn. residues / 84961-70-6 / 284-660-7
Being a multiconstiuent substance, several peaks were observed. The log Pow for each fraction was 8.61, 9.05, 11.44, 11.56, 11.87, 11.93, 12.04, 12.37, 12.42, and 12.53.
3. OECD Guideline 117
Test material information: Benzene, mono-C10-13-alkyl derivs., distn. residues / 84961-70-6 / 284-660-7
Details on results: Being a multiconstiuent substance the log Pow for each fraction was 6.67 and 6.82.

7.5. Manufacture and uses

7.5.1. Quantities

Table 8

AGGREGATED TONNAGE (PER YEAR)				
☐ 1 – 10 t	☐ 10 – 100 t	☐ 100 – 1000 t	☐ 1000- 10,000 t	☒ 10,000-50,000 t
☒ 50,000 – 100,000 t	☐ 100,000 – 500,000 t	☐ 500,000 – 1000,000 t	☐ > 1000,000 t	☐ Confidential

7.5.2. Overview of uses

This substance is used by consumers, in articles, by professional workers (widespread uses), in formulation or re-packing, at industrial sites and in manufacturing.
Based on Registrant(s)' communication, eleven industrial uses are identified with the substance HAB as: closed system oil, industrial functional fluid, lubricants and greases (in open and closed systems), production of polymers or rubber products, fuel additive, metal and non-metal surface treatment, ink and toners, paints and coatings, extraction agent and in washing and cleaning product.

The Registrant(s) provided a CSR with 15 exposure scenarios (ES) for industrial use that are divided in sub-scenarios, corresponding principally to the specific Environmental Release Categories (ERCs) with specific release fractions.
Based on costumer communication, eleven industrial uses are identified. Uses include use as closed system oil, use as industrial as industrial functional fluid, use as lubricants and greases (in open and closed systems), use for the production of polymers or rubber products, use as fuel additive, use as metal and non-metal surface treatment, use in ink and toners, use in paints and coatings, use as extraction agent and use in washing and cleaning product.

A total of 14 professional wide dispersive uses have been identified. HAB is used professionally in closed system oils, in lubricating oils in closed and open system, in rubber and mastics, paintings and coatings, as washing and cleaning products, in concrete and asphalt concrete, as laboratory chemical, in ink, toners, dyes, finishing and impregnation products, as adhesive/sealant, polished and wax blends, in welding and soldering products and flux products, as extraction agent, in fuels and in agrochemicals.

Table 9

USES	Use(s)
Uses as intermediate	See below

Formulation	This substance is used in polymers, polishes and waxes, adhesives and sealants, lubricants and greases, heat transfer fluids, metal working fluids, washing & cleaning products, non-metal-surface treatment products and leather treatment products. Release to the environment of this substance can occur from industrial use: formulation of mixtures, formulation in materials, manufacturing of the substance, in processing aids at industrial sites, in the production of articles, as an intermediate step in further manufacturing of another substance (use of intermediates), as processing aid and of substances in closed systems with minimal release. Other release to the environment of this substance is likely to occur from outdoor use as processing aid.
Uses at industrial sites	Eleven industrial uses are identified with the substance HAB. This substance is used in lubricants and greases, heat transfer fluids, washing & cleaning products, metal working fluids, fuels, non-metal-surface treatment products, polymers, coating products, inks and toners, extraction agents and polishes and waxes. This substance is used in formulation of mixtures and/or re-packaging. This substance is used for the manufacture of chemicals. Release to the environment of this substance can occur from industrial use: in processing aids at industrial sites, of substances in closed systems with minimal release, in the production of articles and as an intermediate step in further manufacturing of another substance (use of intermediates).
Uses by professional workers	A total of fourteen professional wide dispersive uses have been identified. This substance is used in lubricants and greases, washing & cleaning products, polishes and waxes, adhesives and sealants, heat transfer fluids and biocides (e.g. disinfectants, pest control products). This substance is agriculture, forestry and fishing, formulation of mixtures and/or re-packaging and mining. This substance is used for the manufacture of chemicals, plastic products and rubber products. Other release to the environment of this substance is likely to occur from outdoor use, indoor use (e.g. machine wash liquids/detergents, automotive care products, paints and coating or adhesives, fragrances and air fresheners) and outdoor use in close systems with minimal release (e.g. hydraulic liquids in automotive suspension, lubricants in motor oil and break fluids)
Consumer Uses	This substance is widespread used in washing & cleaning products, lubricants and greases and fuels. Other release to the environment of this substance is likely to occur from indoor use (e.g. machine wash liquids/detergents, automotive care products, paints and coating or adhesives, fragrances and air fresheners), outdoor use, outdoor use in close systems with minimal release (e.g. hydraulic liquids in automotive suspension, lubricants in motor oil and break fluids) and indoor use in close systems with minimal release (e.g. cooling liquids in refrigerators, oil-based electric heaters).
Article service life	Other release to the environment of this substance is likely to occur from outdoor use in long-life materials with low release rate (e.g. metal, wooden and plastic construction and building materials) and outdoor use in long-life materials with high release rate (e.g. tyres, treated wooden products, treated textile and fabric, brake pads in trucks or cars, sanding of buildings (bridges, facades) or vehicles (ships)). This substance can be found in products with material based on rubber (e.g. tyres, shoes, toys).

7.6. Classification and Labelling

7.6.1. Harmonised Classification (Annex VI of CLP)

The substance is not currently listed on Annex VI of CLP Regulation ((EC) No 1272/2008).

7.6.2. Self-classification

- In the registration:

Asp. Tox. 1 H304: May be fatal if swallowed and enters airways

7.7. Environmental fate properties

7.7.1. Degradation

Studies regarding stability in water (hydrolysis) or in light (phototransformation/ photolysis) of HAB are not available. However, on the basis of structure and physical-chemical properties, it is assumed that the abiotic degradation of the substance would not contribute significantly to the depletion of the substance within the environment.

Biodegradation

Table 10 Screening tests for biodegradation in water provided by Registrant(s):

Method	Results	Remarks
biodegradation in water: ready biodegradability: activated sludge (adaptation not specified) (aerobic) according to BODIS - Test (BOD-test for insoluble substances)	poorly biodegradable % Degradation of test substance: 28 after 28d (% degradation (O2 consumption))	1 (reliable without restriction) key study experimental study Test material HAB (CAS: 84961-70-6 EC 284-660-7). Reference Schober 1993

The key study was conducted to examine the potential of the test substance to biodegrade using the BODIS test for insoluble substances. Samples of activated sludge were exposed to 5.4, 5.8, and 6.0 mg/flask of the test substance. Diethylene glycol was used as the reference substance. Oxygen measurements were taken at 7, 14, 21, and 28 days. The test substance degraded 28% by the end of 28 days. Therefore, the study demonstrates that HAB **does not meet the criteria for ready biodegradability.** eMSCA agreed with the Registrant(s) conclusion.

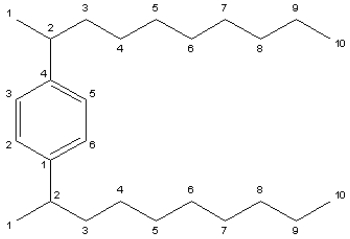
As requested in the Substance Evaluation Decision, the Registrant(s) submitted a soil simulation testing with reliability 1 (unpublished study report, 2019), performed with **1,4-di(2-decanyl)benzene**, a specific surrogate substance, considered representative of the major category (**dialkyl benzenes**) and of the whole registered substance. The study was carried out according to the OECD guideline 307 (Aerobic and anaerobic transformation in soil) and in compliance with GLP.

Aerobic and anaerobic transformation studies were run for 120 days (in the anaerobic testing, there was a 28 day aerobic exposure period prior to the 120 day anaerobic exposure period) using four different soils. The studies of radiolabelled 1,4-di-(2-decanyl)benzene were conducted at 20 °C with initial concentrations of 5.17 µCi/vessel for the anaerobic biodegradation and 4.55 µCi/vessel for the aerobic one. NaOH traps were used to determine the amount of CO_2 evolved, and ethylene glycol traps were used to measure the amount of organic volatiles produced. At the end of the 120 days in the aerobic biodegradation study the amount of CO_2 evolved ranged from 25.6 to 37.2% and the test substance ranged from 31.2 to 54.1%. At the end of the anaerobic transformation study the range of CO_2 evolved was 5.1 - 10.7% and the test substance ranged from 77.3 to 88.1%. Non-extractable residues (NER) ranged from 12.8 to 21.8% in the aerobic study, and 4.3 - 9.1% in the anaerobic trasformation. No volatile organic compounds were

detected in both studies. The total unidentified radioactivity in the extractable residues ranged from 1.3% to 4.4% in the aerobic test.

Half-lives for the substance in the aerobic testing ranged from 23 to 178 days at 20 °C. When the results were adjusted for 12 °C using the Arrhenius equation, the half-lives ranged from 49 to 378 days. Anaerobic degradation was significantly slower with half-lives ranging from 1114 to 6.3E+09 days and 2365 to 1.3E+10 days at 20 °C and 12 °C, respectively.

Reference substance: [phenyl-14C-U]1,4-di(2-decanyl)benzene
CAS name**: Benzene, 1,4-bis(1-methylnonyl)-**
Molecular formula: C26H46
Molecular weight:360.64
SMILES notation: CCCCCCCCC(C)c1ccc(cc1)C(C)CCCCCCCC
Structural formula:



1,4-di(decan-2-yl)benzene

The Registrant(s) concluded that the test substance degraded slowly under aerobic conditions, and even more slowly under anaerobic conditions. Based on the available information, the eMSCA can support this conclusion.

Concerning simulation testing for biodegradation in water and sediment the Registrant(s) proposed a data waiving since the soil simulation testing indicates that the registered substance would be considered persistent/very persistent. eMSCA agrees with the Registrant(s) justification and considers acceptable the proposed waiver for the purpose of the substance evaluation.

Estimated data

The Registrant(s) analyzed representative structures from each category of components identified in HAB using the BIOWIN model (v4.10) found in the US EPA's EPISuite (v4.11) group of QSAR models. The results were then compared to the persistency screening criteria found in the European Commission 2003 Technical Guidance Document on Risk Assessment and Guidance on Information Requirements and Chemical Safety Assessment Chapter R.11: PBT/vPvB assessment. Based on the TGD criteria, 5 of the 21 categories would be considered persistent. Using the criteria in Guidance Chapter R.11, 5 categories would be considered potential persistent, very persistent and an additional 12 would be considered borderline.

eMSCA reports below the outcome of the BIOWIN 2, 3 and 6 models, performed for each constituent type. The results confirm the Registrant(s) conclusion.

Table 11

Type	**BIOWIN 2**	**BIOWIN 3**	**BIOWIN 6**	**CONCLUSION** **2 and 3 or** **6 and 3** *Does not biodegrade fast (probability < 0.5) and ultimate biodegradation timeframe prediction: ≥ months (value < 2.25 (to 2.75))*
1) dialkyl benzenes	0.8766	2.7296	0.3466	border-line

2) trialkyl benzenes	0.8799	2.5811	0.1905	border-line
3) alkyl dialkyl benzenes	0.9656	2.7787	0.1426	
4) monoalkyl benzenes	0.9765	2.9001	0.5446	
5) alkylindanes	0.9510	2.7212	0.2488	border-line
6) Alkyl Tetra-hydronaphthalenes	0.9510	2.7212	0.2488	border-line
7) Alkyl Alkylene Benzenes	0.9724	2.8142	0.0716	
8) Alkyl Octahydroanthracenes	0.9726	2.6508	0.1286	border-line
9) Alkylindenes	0.9181	2.8005	0.1798	
10) Alkyl Dialkyl Dihydronaphthalenes	0.9424	2.6946	0.1636	border-line
11) Alkyl Tetraalkyl Dihydronaphthalenes	0.8981	2.4338	0.0194	border-line
12) Alkyl Alkylene Dihydronaphthalenes	0.9829	2.7366	0.0093	border-line
13) Alkylnaphthalenes	0.9455	2.5506	0.0211	border-line
14) Diphenyl Alkanes	0.8042	2.2102	0.0834	Potentially P or vP
15) Alkyl Diphenyl Alkanes	0.7933	1.9637	0.0036	Potentially P or vP
16) AlkylAcenaphthenes	0.9793	2.5422	0.0161	border-line
17) Phenyl Alkyl Tetra-hydronaphthalenes	0.8827	2.1398	0.0469	Potentially P or vP
18) Phenyl Alkyl Indanes	0.9181	2.2018	0.0537	Potentially P or vP
19) Alkyl Phenyl Alkylene Benzenes	0.9181	2.2018	0.0537	Potentially P or vP
20) Alkyl Acenaphthylenes	0.9389	2.6964	0.0153	border-line
21) Alkyl Fluorenes	0.7381	2.4097	0.0370	border-line

7.7.2. Environmental distribution

No experimental studies investigating the adsorption/desorption behaviour of Benzene, mono-C10-13-alkyl derivs., distn. residues are available. EPI Suite v3.1 adsorption/desorption modelling was conducted for five representative compounds: p-bis (1 -methylundecyl) benzene, mp-bis 2,9-diphenyldodecane, 1-methyl-5-(1-methylundecyl)-2-(1-pentyl)benzene, 1,4-dipropyl-6-(1-methylundecyl)-tetralin, and 1,4-dihydro-1,4-dipropyl-6-(1-methylundecyl)-naphthalene, with calculated soil Koc values of 2.7E8, 7.9E6, 2.0E6, 5.7E7 and 5.7E7, respectively.

Based on vapour pressure value, HAB is not expected to significantly volatilize to air.

Level III fugacity modelling conducted on five representative constituents with the EPI Suite (USEPA 2000, 2007) indicates that these materials will distribute primarily to soil or sediment.

7.7.3. Bioaccumulation

Registrant(s) provided one experimental study and 21 BCF values estimated by QSARs.

Experimental study

The reported BCF (aquatic species) is 35 L/kg ww deriving from the experimental test on **Monoalkylbenzene - LAB** (Werner, AF, and Kimerle, RA, 1982) according to ASTM Committee E-35.21.Test material information is reported below:

Benzene, C10-C13 Alkyl derivs.
EC number 267-051-0
CAS RN 67774-74-7

Undecylbenzene
Molecular Formula C17H28
MW: 232.4
EC number 229-806-2 EC
CAS RN 6742-54-7
SMILES CCCCCCCCCCCC1=CC=CC=C1

This experimental test examined the bioaccumulation of **linear alkylbenzenes** in fish. 150 bluegill fish were exposed to 0.092 mg/L (0.1 mg/L nominal) of test substance for 96 hrs (flow-through test). A steady state concentration in fish was reached at 48 hrs. Samples were analyzed using liquid scintillation counting. During the depuration phase, the fish were sampled at 2, 4, 8, 24, 48, 72, and 96 hrs. An additional 150 fish were exposed to vehicle (acetone). Tissues concentrations at 96 hrs were 115 µg/g in the gall bladder, 7.1 µg/g in the viscera, and 1.3 µg/g in the remainder of the fish. Using the steady state method, no significant differences were seen in whole fish concentrations of test materials in three 24 hr sampling intervals. The depuration phase lasted until 10% of the steady state concentration was reached in fish. Calculation of the uptake and depuration rates was done using the BIOFAC method.
The plateau method was used to determine the BCF values. The bioaccumulation factor in fish was 35 L/Kg.

QSAR calculations

In their updated dossier, the Registrant(s) reported also QSAR calculations (EPISUITE) of representative constituents of the UVCB substance in order to analyse B properties of concern. The Registrant(s) concluded that modelled BCF values of all representative constituents indicate no concern for bioaccumulation of the registered substance.
With respect to the Registrant(s) conclusion on bioaccumulation potential of the registered substance, eMSCA notes that the prediction could be relevant just for some categories of constituents.

eMSCA is aware that the registered substance is an extremely complex hydrocarbon UVCB and it is characterized by 21 different categories of components. "The total number of individual components is estimated to be nearly 1000. It has been estimated that there are 210 possible isomers in the category of dialkyl benzenes alone. The categories are: 1) dialkyl benzenes, 2) trialkyl benzenes , 3) alkyl dialkyl benzenes, 4) monoalkyl benzenes, 5) alkylindanes, 6)Alkyl Tetra-hydronaphthalenes, 7) Alkyl Alkylene Benzenes, 8) Alkyl Octahydroanthracenes, 9)Alkylindenes, 10) Alkyl Dialkyl Dihydronaphthalenes, 11) Alkyl Tetraalkyl Dihydronaphthalenes, 12) Alkyl Alkylene Dihydronaphthalenes, 13) Alkylnaphthalenes, 14) Diphenyl Alkanes, 15) Alkyl Diphenyl Alkanes, 16) AlkylAcenaphthenes, 17) Phenyl Alkyl Tetra-hydronaphthalenes, 18) Phenyl Alkyl Indanes, 19) Alkyl Phenyl Alkylene Benzenes, 20) Alkyl Acenaphthylenes and 21) Alkyl Fluorenes."

According to ECHA guidance IR&CSA- Chapter R.11: PBT/vPvB assessment. Version 3.0 – June 2017, for substances containing multiple constituents, impurities and/or additives, the guidance applies to that/those "part(s)" of the substance, which is/are the target of assessment and testing. The criteria for selecting an appropriate assessment approach are provided in Section R.11.4.2.2 (Assessment of substances containing multiple constituents, impurities and/or additives).

eMSCA notes that the Registrant(s) reported SMILES notations and structures for representative components of each category and carried out QSAR calculations (US EPA's EPISUITE v.4.11) for all representative substances of each category. In particular, the QSAR estimations provided by the Registrant(s) are related to: water solubility, $logk_{ow}$, $logk_{oc}$, persistence and BCF/BAF.
eMSCA agrees with Registrant(s) that standard tests for this endpoint are intended for single substances and are not appropriate for this complex substance. Further complicating the potential bioaccumulation testing of HAB constituents is the extremely low water solubility (WATERNT estimates from 2.61e-03 to 5.83e-07 mg/L) and extremely high $logK_{ow}$ (KOWWIN estimates from 7.87 to 19.62) of the individual components. Following the PBTEG comments, it was noted that the high hydrophobicity is expected to result in a slow uptake kinetic for HAB components. A slow uptake kinetic might indicate a low bioavailability. However, a slow uptake could also lead to a slow bioaccumulation process and in some cases anyway this may lead to a high BCF value in long-term. (Larisch, W., Goss, K.-U., 2018). Indeed, eMSCA cannot exclude that these substances might slowly bioaccumulate over time and eventually result in a high BCF value in long-term. In this respect, especially for such high $logK_{ow}$ values (>10), the current knowledge does not allow to discriminate slow bioaccumulation processes and to derive a reliable BCF according to OECD 305 TG.

About the estimation of the applicability and accuracy of KOWWIN model, eMSCA highlights that all the substances considered in the calculations have a MW range of 246.44-583.09 and the fragments included in the model completely cover the structural formula. Therefore, the substances fall within the applicability domain of the QSAR model.

Based on the $logk_{ow}$ values predicted by KOWWIN model for the selected individual structures, it can be stated that only the substance representative for **monoalkyl benzenes LAB category** (CAS 2719-61-1) has a $logk_{ow}$ value of 7.87, whereas the other substances have $logk_{ow}$ values exceeding 10.
According to ECHA Guidance R.11 these predictions should be considered in qualitative terms i.e. they are not to be used as a QSAR to estimate BCF from $logK_{ow}$. As described in Appendix R.11—1: *Indicators for limited bioconcentration for PBT assessment* - Annex 1 (*Development of a $logk_{ow}$ cut-off value for the b-criterion in the pbt-assessment*), based on the current limited knowledge (both with respect to measured $logK_{ow}$ and BCFs), a calculated $logK_{ow}$ of 10 or above is taken as an indicator for showing reduced bioconcentration. However, a $logK_{ow}$ value higher than 10 should be used in a Weight-of-Evidence approach in combination with other indicators.

About the BCF estimations, eMSCA notes that for BCF-Regression model with BCFBAF model (EPISUITE), all the molecular weights fall within the range of the training sets, all fragments of the substances were analysed, but only some $logK_{ow}$ values of Category Representatives fall within the training set's range (**monoalkyl benzenes, alkyl alkylene benzenes** and **akyl phenyl alkylene benzenes**). In particular, for these substances, the calculated BCF values are largely below < 2000.
In all other cases the $logK_{ow}$ values of Category Representatives fall outside the training set's range.
In particular, regarding Arnot-Gobas model, the predictions should be considered highly uncertain for most of the individual Category Representatives considered by the Registrant(s) due to $logk_{ow}$ values > 9. Only the monoalkyl benzenes category-LAB (Category Representative CAS: 2719-61-1, $logk_{ow}$= 7.87) has an estimated reliable BCF. The results obtained (including biotransformation rate estimates) for upper trophic, middle trophic and lower trophic fish are very low (880 and 151 L/Kg).

Moreover, the Registrant(s) indicated that there is a measured BCF value of 35 L/Kg in Bluegill Sunfish, confirming that there are no bioaccumulation concerns for this category (monoalkyl benzenes). eMSCA raises doubts on the reliability of this available experimental bioaccumulation outcome: no lipid normalization was indicated; the uptake rate constant was too low; the BCF-test had been performed above the water solubility (nominal and measured concentrations of 0.1 mg/L and 0.092 mg/L respectively). Moreover undecylbenzene / 6742-54-7; 229-806-2 was used as test material. The QSAR estimation (EPISUITE v.4.11) for this substance led to BCF values in the range = 188.4- 2905 L/kg wet-wt. Registrant(s) claimed that the experimental value is lower than the estimated ones due to the supposed rapid metabolism.
eMSCA notes that monoalkyl benzenes, dialkyl benzenes and trialkyl benzenes are the most abundant categories for the registered UVCB. In light of QSAR estimations above reported, eMSCA highlights the following conclusion. The $logk_{ow}$ values >10 for the most of representative structures from each category of UVCB (including dialkyl benzenes) and very low estimated BCF values obtained for monoalkyl benzene category are relevant just for a weight of evidence approach.
Table 12 shows results of BCF estimations by QSAR models US EPA's EPISUITE v.4.11 provided by Registrant(s). The categories within training set range are highlighted in bold.

Table 12

Constituents/categories	BCF (regression-based model)	BCF (Arnot-Gobas upper trophic)	Remarks
Category Name	All the molecular weights falls within the range of the training sets (68.08 to 959.17) and all fragments of the substances were analysed		
1) dialkyl benzenes	7	1	MW of Category Representative 414.77. Its $logK_{ow}$ (13.74) **falls outside** the training set's range (-1.37 to 11.26)
2) trialkyl benzenes	3	1	MW of Category Representative is 583.09. Its $logK_{ow}$ (19.62) **falls outside** the training set's range (-1.37 to 11.26)
3) alkyl dialkyl benzenes	13	1	MW of Category Representative is 358.66. Its $logK_{ow}$ (11.91) **falls outside** the training set's range (-1.37 to 11.26)
4) monoalkyl benzenes	**880**	**151**	MW of Category Representative is 246.44. Also, its $logK_{ow}$ (7.87) **falls within** the training set's range (-1.37 to 11.26)
5) alkylindanes	23	1	MW of Category Representative is 384.69. Its $logK_{ow}$ (12.63) **falls outside** the training set's range (-1.37 to 11.26)
6) Alkyl Tetra-hydronaphthalenes	23	1	MW of the of Category Representative is 384.69. Its $logK_{ow}$ (12.63) **falls outside** the training set's range (-1.37 to 11.26)
7) Alkyl Alkylene Benzenes	**29**	**2**	MW of the Category Representative is 342.61. Its $logK_{ow}$ (11.20) **does not fall outside** the training set's range (-1.37 to 11.26).
8) Alkyl Octahydroanthracenes	27	1	MW of the Category Representative is 382.68. Its $logK_{ow}$ (12.50) **falls outside** the training set's range (-1.37 to 11.26)

9) Alkylindenes	25	1	MW of the Category Representative is 382.68 which falls within the range of the training set. Its $logK_{ow}$ (12.55) **falls outside** the training set's range (-1.37 to 11.26)
10) Alkyl Dialkyl Dihydronaphthalenes	17	1	MW of the Category Representative is 396.71. Its $logK_{ow}$ (12.91) **falls outside** the training set's range (-1.37 to 11.26)
11) Alkyl Tetraalkyl Dihydronaphthalenes	3	1	MW of the Category Representative is 480.87. Its $logK_{ow}$ (15.97) **falls outside** the training set's range (-1.37 to 11.26)
12) Alkyl Alkylene Dihydronaphthalenes	440	25	MW of the Category Representative is 478.85. Its $logK_{ow}$ (15.75) **falls outside** the training set's range (-1.37 to 11.26)
13) Alkylnaphthalenes	3	1	MW of the Category Representative is 563.02. Its $logK_{ow}$ (18.47) **falls outside** the training set's range (-1.37 to 11.26)
14) Diphenyl Alkanes	27	1	MW of the Category Representative is 490.86. Its $logK_{ow}$ (15.38) **falls outside** the training set's range (-1.37 to 11.26)
15) Alkyl Diphenyl Alkanes	3	1	MW of the Category Representative is 490.86. Its $logK_{ow}$ (15.62) **falls outside** the training set's range (-1.37 to 11.26)
16) AlkylAcenaphthenes	3	1	MW of the Category Representative is 532.94. $logK_{ow}$ (17.36) **falls outside** the training set's range (-1.37 to 11.26)
17) Phenyl Alkyl Tetra-hydronaphthalenes	3	1	MW of the Category Representative is 488.85. Its $logK_{ow}$ (15.25) **falls outside** the training set's range (-1.37 to 11.26)
18) Phenyl Alkyl Indanes	4	1	MW of the Category Representative is 460.79. Its $logK_{ow}$ (14.27) **falls outside** the training set's range (-1.37 to 11.26)
19) Alkyl Phenyl Alkylene Benzenes	**440**	**25**	MW of the Category Representative is 334.55. Also, its $logK_{ow}$ (10.02) **falls within** the training set's range (-1.37 to 11.26)
20) Alkyl Acenaphthylenes	3	1	MW of the Category Representative is 530.93. Its $logK_{ow}$ (17.27) **falls outside** the training set's range (-1.37 to 11.26)
21) Alkyl Fluorenes	20	1	MW of the Alkyl Fluorenes Category Representative is 390.66. Its $logK_{ow}$ (11.56) **falls outside** the training set's range (-1.37 to 11.26)

Based on the available information, the BCF values estimated with BCFBAF QSAR models suggest a low bioaccumulation of the 21 categories/fractions of the UVCB substance.
Based on the $logk_{ow}$ values predicted by KOWWIN model for the selected individual structure representatives of the 21 categories/fractions, only the substance (**monoalkyl benzenes LAB, CAS 2719-61-1)** has a $logk_{ow}$ value of 7.87, whereas the other substances have $logk_{ow}$ values exceeding 10.

Indeed the indication of a low bioaccumulation potential is only met for substances with a $logK_{ow}$ in excess of 10. Moreover, the QSAR models US EPA's EPISUITE v.4.11 provides

BCF =880 L/Kg (regression-based model) and BCF = 151 L/Kg (Arnot-Gobas upper trophic) for group of monoalkylbenzenes. The calculated $logK_{ow}$ of the monoalkylbenzenes falls within the applicability domain. eMSCA is aware that alone this information is not sufficient to conclude on B for the whole substance. However, considering the fraction profiling according to the Chapter R.11 of ECHA Guidance, at least for the all fractions with reliable $logK_{ow}$ > 10, no indication of potential B remains.
According to ECHA Guidance R.11 these predictions should be considered in qualitative terms i.e. they are not to be used as a QSAR to estimate BCF from $logK_{ow}$. eMSCA notes also that that for BCF-Regression almost all $logK_{ow}$ values of Category Representatives fall outside the training set's range (-1.37 to 11.26).
For what concern the BCF estimated by QSAR, the only case with an estimated $logK_{ow}$ value in the range of $logK_{ow}$ 7.87 (Category Representative monoalkyl benzenes LAB, CAS 2719-61-1) the results obtained are very low (880 and 151 L/Kg).

Additional information on field studies on bioaccumulation of C11-14 LABs in mussels and fish was provided during the written procedure of PBTEG discussion. It was suggested that the position of the phenyl group implicates a difference in bioavailability for degradation, and could also have an influence in the uptake and metabolism of the different LAB isomers. Authors (Bayona et al. 1986) showed that degradation was slower when the phenyl group was closer to the center of the chain and the higher isomers.
Philips et al (2001) have measured C11-C14-LAB isomers in fish and mussels. Murray et al (1991) in a field study with *Metylus edulis* indicated that values for the total LABs were similar to PAHs, e.g. as B(a)P, which are classified as vB.
Based on the table presented by Philipps *et al.* (2001) it seems the LABs would accumulate at a higher concentration in molluscs than in fish, similarly to PAHs. This higher accumulation could be due to the lower metabolism capacity of molluscs. Similar results were shown by Dwiyitno *et al.* (2016) who measured higher concentration of LABs in mussels as compared to fishes. In all cases, the feeding mode and associated suspended particles seem to be relevant for the uptake.
The above information are relevant just to indicate that high LABs levels were detected in the biota (mussel and fish species) and present in the different investigated areas . According to eMSCA, it is very difficult to compare bioconcentration factors in field studies with the standard BCF foreseen by OECD 305 TG, mainly due to variability in exposure conditions, experimental methodology and reporting data, not in compliance with the OECD 305 TG. Therefore, also these information should be considered in qualitative terms, and a conclusion on B cannot be reached based only on monitoring data.
eMSCA concludes that all the available information are part of a Weight of Evidence that do not allow to confirm the Registered UVCB substance to fulfil the criteria for B/vB according to Annex XIII criteria.

7.8. Environmental hazard assessment

7.8.1. Aquatic compartment (including sediment)

Short-term aquatic toxicity data are available for three trophic levels (fish, invertebrates and algae); long-term data are available for two trophic levels (invertebrates and algae). These Studies show that HAB is generally considered to be non-toxic to aquatic organisms at the limits of water solubility.

7.8.1.1. Fish

Short-term toxicity to fish

The Registrant(s) provide two short-term studies based on Read Across (RAA).
The first is a key study (Anon, 2005) with reliability 2 (with restrictions) on *Pimepales promelas*; it is a semi-static study performed according to USEPA Method 2000.0, ASTM E729-96. The substance utilized in read across is V-154L Specialty Alkylate. Duplicate groups of 10 fish were exposed to concentrations of 0, 12.5, 25, 50, 100 % water accommodated fraction (WAF) of test substance. Fish were exposed for 96 hrs, with the

renewal of the test solution at 48 hrs. The 96-hr LC_{50} is > 100% WAF. Based on the experimental reliable data, no toxic effects of HAB were observed on fishes.
The second is a supporting study (Anon, 1999) with reliability 1 on *Danio rerio;* it is a semi-static test performed according to OECD Guideline 204 (Fish, Prolonged Toxicity Test: 14-day Study), GLP. The substance utilized in read across is European commercial linear alkyl benzene (LAB). Fish were exposed for 14 days to a water accommodated fraction of 0.005, 0.0065, and 0.01 mg/L of test substance. The LC_{50} was > 0.01 mg/L. The Registrant(s) concluded that no adverse effect was seen during the study period.
For the key study, eMSCA notes that these studies are not adequately described in accordance with the conditions for the validity of the test. Deficiencies in the information provided were noted. However, no acute toxic effects resulted within the range of solubility. Based on the available information, the eMSCA can support the above conclusion.
For the supporting study, in addition to the deficiencies in the information provided, eMSCA noted that following the OECD Council decision, the test performed according to OECD Guideline 204 (Fish, Prolonged Toxicity Test: 14-day Study), was deleted on 2nd April 2014, and therefore it cannot be considered acceptable.

Long-term toxicity to fish

The Registrant(s) provide a justification for waiving long-term studies on fish, claiming that no toxicological effects in the acute test on fish at the limit of water solubility is noted: *"A 14-day study in Brachydanio rerio showed no effects at any concentration. A longer duration study is therefore not needed."*
eMSCA agrees with the waiving but do not agree with the justification provided by the Registrant(s).
According to Regulation EC 1907/2006, Annex IX, column 2, section 9.1, the long term aquatic toxicity study on fish shall be considered if the chemical safety assessment according to Annex I indicates the need to investigate further the effects to aquatic organisms. Since the aquatic invertebrates tests on C10-14 LAB already clarify the toxicity of the substance for aquatic organisms, and in view of the major sensibility of *Daphnia sp.* gathered from the tests' results, eMSCA do not consider the need of a long-term test on fish.
According to ECHA Guidance on information requirements and chemical safety assessment, Chapter R.7B: *"Tests performed according to OECD 204 or similar guidelines cannot be considered suitable long-term tests. They are in effect prolonged acute studies with fish mortality as the major endpoint examined."* Moreover, as noted above, the test performed according to OECD Guideline 204 (Fish, Prolonged Toxicity Test: 14-day Study), was deleted by OECD on 2nd April 2014, and therefore it cannot be considered acceptable anymore.
Therefore, the Registrant(s) are suggested to revise the waiving according to the recommendations of the eMSCA.

7.8.1.2. Aquatic invertebrates

Two study on *Daphnia magna* were provided by the Registrant(s): one key study and one supporting study according OECD Test Guideline 202 (Acute Immobilisation Test, 1984).
In the key study (Scholz, 1992), static test with reliability 1, organisms were exposed to concentrations of 0.35, 0.49, 0.7, 0.98 and 1.40 mg/L of the registered substance (Benzene, mono-C10-C13 alkyl derivates, distillation residues). The EC_{50} 48h was > 1.4 mg/L (based on nominal concentration), which is greater than the water solubility of the the substance (<0.1 mg/L).
In the supporting study (Fernandez, 2002), semi-static test with reliability 2 with restrictions (RA from supporting substance – Linear Alkyl Benzenes with varying phenyl positions), organisms were exposed to concentrations of 0.0125, 0.025, 0.05 and 0.1 mg/L of the test substance for 144 hrs. Results for phenyl-C10 (the most water soluble HAB component), shows that the EC_{50} 48-96h values were higher than the water solubility limit (0.0404 mg/L), while the extended 120-144 h EC_{50} values were below estimated water solubility limit; therefore, the EC_{50} 48h is > 0.1 mg/L (based on nominal concentration).
According to eMSCA, the condition for validity of the test of key study are fulfilled, despite some information are missing. Also with regard the supporting study, eMSCA notes that a

lot of study information are missing. However, no acute toxic effects resulted within the range of solubility.
Based on the available information, eMSCA can support the above conclusion.

Long-term toxicity to aquatic invertebrates

There are two studies determining the chronic toxicity of LAB (the most water soluble fraction of the HABs) to *Daphnia magna*.
The first is a key study (Minderhout, Gallagher and Krueger, 2013), with reliability 2 (with restriction) according to OECD Guideline 211 (Daphnia magna Reproduction Test); it is a semi-static test where organisms were exposed to LAB, C10-13 (Benzene, C10-13 alkyl derivs – CAS n. 67774-74-7) at nominal WAF loading rates of 0.01, 0.1,1 and 10 mg/L for 21 days. There was no statistically significant treatment related effects on survival, reproduction or growth at concentration ≤ 10 mg/L: the NOEL 21d was = 10 mg/L. Due to the low water solubility of the test substance, no test substance was detected in the analytical monitoring and therefore the results are reported as a WAF (nominal concentration). Based on these results, the Registrant(s), concluded that LAB does not show chronic aquatic toxicity, eMSCA can support the above conclusion.
The second is a supporting study (Gledhill et al., 1991), with reliability 2 (with restriction), based on a flow-through test system, on Daphnia magna according to ASTM E35.21 test guideline, Draft 5 (Proposed Standard Practice for Conducting Renewal Life Cycle Toxicity Tests with Daphnids). This study is reported as a read-across (RAA) from supporting substance (structural analogue or surrogate – Test material C10-14 LAB; tridecylbenzene - CAS n. 68648-87-3), using acetone as a solvent. Daphnids were exposed to concentrations of 0.0019, 0.0038, 0.0075, 0.015 and 0.03 mg/L of test substance. The 21-days NOEC was= 0.0075 mg/L (based on nominal concentrations) (LAB is the most water soluble fraction of HAB).
Although, both in the technical dossier and in the CSR, a reference is made to the OECD SIDS Initial Assessment Report (OECD, 2008), regarding Linear Alkylbenzene (LAB) Alkylate Bottoms Category, there is no justification for RAA and for category approach in the technical dossier (any attached supporting document) nor a Reporting Format for the analogue approach or the chemical category in the CSR.
Despite the above considerations, based on OECD SIDS Initial Assessment Report (OECD, 2008), eMSCA accepts RAA for this endpoint.
Concerning this supporting study, the Registrant(s) concluded (IUCLID file), that the results can be considered conservative as the solvent concentration (1 mL/L) was above the currently recommended levels for solvent addition (<0.1mL/L).

According to OECD GD 23 “The choice of solvent will be determined by the chemical properties of the test chemical and the availability of data to demonstrate that the solvent does not affect the outcome of the study for a given test guideline and species. [...] The concentration of the solvent in the test solution should not exceed the corresponding toxicity thresholds determined for the solvent under the test conditions. The suggested level is at least one order of magnitude below the appropriate no-observed effect concentration (NOEC) depending on the test species and the length/type of toxicity test or in any case below 100 mg/L or 0.1 mL/L (Green and Wheeler, 2013).”
Base on the information at the ECHA dissemination website on acetone (EC 200-662-2), Following the PBTEG suggestions, eMSCA aknowledged that the concentration of acetone used in the study with LAB is near one order of magnitude below the NOEC of acetone (28-day NOEC based on reproduction 2212 mg/L (flow-through test system); 21-day NOEC based on reproduction was >= 79 mg/L (semi-static test)).
Base on this consideration, it would seem that the concentration of acetone in the available test (Gledhill *et al.*, 1991) was one order of magnitude below the NOEC or close to, according to OECD 23.
However, eMSCA notes several shortcomings that raise doubts about the relevance of this supporting study. Indeed there is a general lack of information on the test method ASTM E35.21 test guideline, Draft 5 (Proposed Standard Practice for Conducting Renewal Life Cycle Toxicity Tests with Daphnids) that is not equivalent to the standard OECD TG 211 and it is not among the methods indicated by the ECHA Guidances. The ECHA Guidelines R.7 states that NOEC values from long-term toxicity testing on Daphnia sp. can be used

according to OECD 211 or equivalent test guidelines. Moreover the Key study based on the OECD TG 211 is performed using the most suitable WAF approach, as foreseen by OECD GD 23 for test material with low water solubility.

Due to the above uncertainties for the supporting study, eMSCA considers the registered HAB having not adverse long-term effects on *Daphnia magna* within water solubility range, based on outcome of the Key study (Minderhout, Gallagher and Krueger, 2013).

7.8.1.3. Algae and aquatic plants

One key study with reliability 1 (Scholz, 1993), static on *Desmodesmus subspicatus*, according to OECD Guideline 201 (Alga, Growth Inhibition Test), was provided by the Registrant(s). Algae were exposed for 72 hrs to concentrations of 0.23, 0.39, 0.69, 01.16 and 2.08 mg/L of the registered substance (HAB). EC_{50} 72h (ErC_{50} and EbC_{50}) and NOEC 72h resulted > 2.08 mg/L and ≥ 2.08 mg/L respectively, based on nominal concentration. Both effect values are greater than the limit of water solubility.

According to eMSCA, this study is adequately described and is in accordance with the condition for the validity of the test.

7.8.1.4. Sediment organisms

In the dossier, the Registrant(s) provided a justification for sediment compartment waiving according to the study technically not feasible because the substance is an extremely complex hydrocarbon UVCB and it is comprised of 21 different categories of components and nearly 1000 individual components. Standard tests for this endpoint are intended for single substances and are not appropriate for the risk assessment of this complex substance. Further complicating the sediment testing of HAB is the extremely low water solubility, extremely high $logK_{ow}$ and extremely high $logK_{oc}$ of the individual components. These properties indicate that the test could be tightly bound to organic material in soil and sediments and could have little, if any, bioavailability.
In spite of this, sediment organisms can be exposed via their body surfaces to substances in solution in the overlying water and in the pore-water and to bound substance by direct contact or via ingestion of contaminated sediment particles. For strongly adsorbing or binding substances, preference should be given to test designs and test organisms that cover the exposure via sediment ingestion, as this is the most relevant exposure route for such chemicals.

Based on above considerations, sediment organism toxicity cannot be excluded.

However the Registrant(s) also indicated that the lack of bioavailability can be observed in the results from the recent OECD 222 earthworm reproduction study conducted as a requirement for CoRAP. In the study, concentrations of HAB of up to 1000 mg/kg (dry soil) had no effect on any of the measured endpoints (adult mortality, adult body weight, juvenile production). This resulted in NOECs of 1000 mg/kg (dry soil) and EC_{10s} of >1000 mg/kg (dry soil).
However, in accordance with Annex X (9.5.1 – column 2) *"Long-term toxicity testing shall be proposed by the* Registrant(s) *if the results of the chemical safety assessment indicate the need to investigate further the effects of the substance and/or relevant degradation products on sediment organisms. The choice of the appropriate test(s) depends on the result of the chemical safety assessment."* Therefore the Registrant(s) should change waiving justification on the ground of exposure consideration and not according to the chemical and physical properties.

7.8.1.5. Other aquatic organisms

No relevant information available.

7.8.2. Terrestrial compartment

In order to clarify the initially identified concern on potential risk for soil compartment, the Registrant(s) provided reliable toxicity data for all three terrestrial taxonomic groups (soil macroorganisms, soil microorganisms and terrestrial plants) on HAB.
In particular, as requested under Substance Evaluation Decision, the Registrant(s) submitted the following long term toxicity testing, an OECD 222 earthworm reproduction study, an OECD 208 terrestrial plants, growth test and an OECD 216 soil microorganisms-nitrogen transformation study, with the aim to evaluate the hazard of the registered substance for soil organisms and, accordingly, to derive a conclusive PNEC soil and a related proper characterization of the risk for soil compartment.

In this context, it may be relevant to point out that these test requests were justified as necessary data taking into account that HAB is regarded as an extremely complex hydrocarbon UVCB, including 21 different categories of components, with extremely low water solubility and a very high adsorption to organic material in soil, indicating potential conditions for exposure to the organisms of soil compartment. Thus, due to the intrinsic properties and the unsuitability of the equilibrium partitioning method (EPM) based screening assessment on the registered substance, these terrestrial toxicity studies have been conducted with the purpose of a conclusive evaluation on the potential expected hazard for soil organisms.

With regards to the newly available terrestrial toxicity dataset, eMSCA noted that the results from the submitted tests are reliable and useful data to demonstrate a generally low toxic effects level on soil organisms, overcoming the initially identified concern for soil hazard.
The most sensitive value obtained from an OECD Guideline 208 Terrestrial Plants, Growth Test, a 21dNOEC of 37 mg/Kg soil dw, was used as key value for the outcome of CSA on hazard of soil compartment.

In view of the refined soil hazard assessment and related risk characterization for any identified uses (with RCRs for soil ≤0.01), eMSCA can conclude that the registered substance is not expected to pose a risk to soil organisms.

Following the assessment, eMSCA considers that newly submitted data on soil organisms as provided by the Registrant(s) are suitable and definitive, fulfilling the requested information under Substance Evaluation Decision.

Therefore, based on the outcome of the revised CSA, eMSCA can support the Registrant(s)' conclusion that effects on soil organisms are not of concern; under this substance evaluation no further information is needed to clarify the hazard on soil organisms and related concern.

<u>Toxicity to soil macro-organisms</u>

As requested in the Substance Evaluation Decision, the Registrant(s) submitted a long-term toxicity study to soil macroorganisms (Sloman T.L. and Porch, J.R.,2017), performed with the registered substance according to the OECD Guideline 222 (Earthworm Reproduction Test (*Eisenia fetida/Eisenia andrei*)) and under GLP.
The toxic effects of HAB on survival, growth and reproduction of earthworms *Eisenia fetida* were assessed during a 56 days exposure period in artificial soil substrate. In this reliable test, adult earthworms were exposed to concentrations of 0, 62.5, 125, 250, 500 and 1000 mg/kg dry soil of test substance for 28 days. The adults were then removed and offsprings were exposed for an additional 28 days.
No statistically significant effects of test substance were observed on earthworms for all measured endpoints (adult mortality, adult body weight, juvenile production).
The EC_{50} of HAB for earthworms was >1000 mg/kg dry soil (nominal) based on adult mortality. The NOECs for growth and reproductive effects (based on number of offspring produced) were 1000 mg/kg dry soil. (nominal).

Based on the experimental reliable data, no toxic effects of HAB were observed on soil macroorganisms.
Therefore, although this substance mainly distributes on terrestrial compartment, based on all newly reliable information on terrestrial toxicity, the CSA indicates that ecotoxicological effects on soil macroorganisms are not of concern.
Following the assessment, eMSCA can conclude that soil macroorganisms data, as provided by the Registrant(s) in the CSR and technical dossier, are suitable and definitive for this endpoint. Consequently, under this substance evaluation, no additional information is needed to clarify the hazard on soil macroorganisms and related concern.

Toxicity to terrestrial arthropods

The registration dossier does not contain data for this endpoint. The Registrant(s) have waived testing on terrestrial arthropods with a justification indicating that toxicity testing on this endpoint is scientifically not necessary. Available toxicity data set on other soil organisms as requested in Substance Evaluation Decision indicates that the registered substance does not show direct toxicity to terrestrial organisms.
Therefore, based on the currently available data, eMSCA can support the Registrant(s)' conclusion on terrestrial arthropods. As such, the outcome of CSA indicates that further assessment of this endpoint is not required.

Toxicity to terrestrial plants

One experimental long term toxicity study (McKelvey, R.A., and Porch, J.R. 2018) has been submitted by the Registrant(s) for this endpoint in order to investigate the toxicity effects of HAB to terrestrial plants, in line with the information request under Substance Evaluation Decision. The study was performed according to OECD Guideline 208 (Terrestrial Plants, Growth Test) and GLP criteria, using ten plants species (four monocotyledonae and six dicotyledonae, respectively). Seeds were planted and exposed to soil containing the registered substance for 21 days, and the emergence and growth of the plants were monitored at any of the following tested concentrations: oilseed rape - 0, 0.457, 1.37, 4.12, 12.3, 37.0 and 111 mg a.i./kg and all other crops: 0, 4.12, 12.3, 37.0, 111, 333 and 1000 mg a.i./kg.
The EC_{50} values of HAB for all test species were greater than the highest concentration tested (111 mg./kg dry soil for oilseed rape and 1000 mg./kg dry soil for all other species). The NOEC values ranged from 37 mg/kg dry soil for Tomato up to 1000 mg/kg dry soil for other species.
In this reliable test, generally low levels of toxicity to all tested terrestrial plants species were observed on all endpoints examined (rate of emergence and growth) over the exposure time.
The test results from this OECD Guideline 208 terrestrial plant toxicity study can be considered as acceptable with all relevant test validity criteria fulfilled.
These submitted data were taken into account for the derivation of PNEC soil as well as for the hazard assessment conclusion on soil organisms. Therefore, following the assessment, eMSCA considers that newly submitted data provided by the Registrant(s) meet the requested information under Substance Evaluation Decision.
Based on the outcome of revised CSA, eMSCA can conclude that there is no indication of concern for effects to terrestrial plants, supporting the Registrant(s)' assessment on this endpoint.

Toxicity to soil microorganisms

As requested in the Substance Evaluation Decision, the Registrant(s) submitted a reliable soil micro-organisms toxicity study (Schaefer, E.C., Wang, N., and Huchler, A.B. 2018) performed according to OECD Guideline 216 and under GLP in order to investigate the effects of the HAB on terrestrial microorganisms.
The test substance was added to soil at a concentration of 1000 mg/kg dry soil and the nitrate formation rate determined after 28 days exposure.
The 28d EC_{50} based on inhibition of nitrate formation rate was determined at >1000 mg/kg dry soil while the 28dNOEC was ≥ 1000 mg/kg dry soil, demonstrating low values of toxicity for soil microorganisms. All validity criteria of the test were fulfilled.

Following the assessment of all newly available data, eMSCA can support the Registrant(s)' conclusions that the effects on soil microorganisms are not of concern.

7.8.3. Microbiological activity in sewage treatment systems

The Registrant(s) report a $PNEC_{STP}$ = 2 mg/L.
The PNEC was calculated using NOEC value of 20 mg/L, derived from BODIS test. The Assessment Factor used is 10. The choice of a AF value of 10 is valid according to ECHA Guidance on information requirements and chemical safety assessment, chapter R10: Characterisation of dose (concentration)-response for environment.
The eMSCA agrees with the Registrant(s).

7.8.4. PNEC derivation and other hazard conclusions

Table 13

PNEC DERIVATION AND OTHER HAZARD CONCLUSIONS		
Hazard assessment conclusion for the environment compartment	**Hazard conclusion**	**Remarks/Justification**
Freshwater	PNEC: 0.001mg/L (CSR) 0.00075 mg/L (IUCLID file) According to eMSCA: PNEC: 0.001mg/L	Assessment factor: 10 (CSR and IUCLID file) from NOEC = 0.0075 mg/L (LAB, most water soluble component) from 21-day *Daphnia magna* study (Gledhill) and AF = 10 from ECHA Guidance -Table R.10-4 According to eMSCA: Assessment factor: 100 EC_{50} > 0.1 mg/L (phenyl-C10, most water soluble single component) from 48-hr *Daphnia magna* study (Fernandez), from ECHA Guidance -Table R.10-4 (see explanation below)
Marine water	PNEC: 0 mg/L (CSR) 0.000075 mg/L (IUCLID file) According to eMSCA: PNEC: 0.0001mg/L	Assessment factor: 100 (CSR and IUCLID file) from NOEC = 0.0075 mg/L (LAB, most water soluble component) from 21-day *Daphnia magna* study (Gledhill) and AF = 10 from ECHA Guidance Table R.10-4 According to eMSCA: Assessment factor: 1000 EC_{50} > 0.1 mg/L (phenyl-C10, most water soluble single component) from 48-hr *Daphnia magna study* (Fernandez) from ECHA Guidance, Table R.10-5 (see below)
Intermittent releases to water	PNEC: 0.001mg/L	Assessment factor: 100 PNEC intermittent release justification: EC_{50} > 0.1 mg/L (phenyl-C10, most water soluble single

		component) from 48-hr *Daphnia magna* study (Fernandez) and AF = 100 from Section R.10.3.3
Sediments (freshwater)	PNEC: 16.5mg/kg sediment dw According to eMSCA: See below	Extrapolation method: equilibrium partitioning method (see below Justification for adaptation of the PNECsediment)
Sediments (marine water)	PNEC: 1.65mg/kg sediment dw According to eMSCA: See below	Extrapolation method: equilibrium partitioning method (see below Justification for adaptation of the PNECsediment)
Sewage treatment plant	PNEC STP: 2mg/L	Assessment factor: 10 Extrapolation method: assessment factor PNEC STP Based on no toxicity at approximately 20 mg/L in BODIS test.
Soil	PNEC soil: 3.7 mg/kg soil dw	Assessment factor: 10 Extrapolation method: assessment factor According to ECHA Guidance R.10, $PNEC_{soil}$ was derived from the lowest NOEC result obtained from an OECD 208 terrestrial plants growth study and an assessment factor of 10. eMSCA can support these soil hazard assessment conclusions, including the related PNEC derivation.

PNEC freshwater

No toxicological effects in the short and long-term test were detected up to and exceeding the water solubility for the registered substance. However eMSCA noted and evaluated the PNEC freshwater reported by the Registrant(s) as cautelative approach, based on the only observed effect on LAB, the most water soluble component of HAB. In addition to the inconsistencies between the CSR and file IUCLID, eMSCA considers that the assessment factor chosen is not correct (AF=10). Indeed, AF=10 is based on the availability of chronic tests for three trophic levels, since the Registrant(s) have considered the test performed according to OECD 204 on fishes as a chronic test. According to ECHA Guidance on information requirements and chemical safety assessment, Chapter R.7B: *"Tests performed according to OECD 204 or similar guidelines cannot be considered suitable long-term tests. They are in effect prolonged acute studies with fish mortality as the major endpoint examined."* Moreover, eMSCA noted that following the OECD Council decision, the test performed according to OECD Guideline 204 (Fish, Prolonged Toxicity Test: 14-day Study), was deleted on 2nd April 2014, and therefore it cannot be considered acceptable as study for the evaluation of acute toxicity neither.

In addition, eMSCA considers incorrect that the calculation of the PNEC is based on NOEC = 0.0075 mg/L, since the validity of the test is questionable for the reason explained above. According to the above arguments, eMSCA considers this study not suitable for the derivation of PNEC.

Taking into account these observations, three acute tests on three trophic levels and two chronic tests on two trophic levels (invertebrates and algae) are available and, therefore, according to Chapter R10, the AF of 100 must be taken into account : "*An assessment*

factor of 100 applies also to the lowest of two long-term results (e.g. EC_{10} or NOECs) covering two trophic levels when such results have not been generated from that showing the lowest L(E)C_{50} of the short-term tests. This should, however, not apply in cases where the acutely most sensitive species has an L(E)C50 value lower than the lowest long term result (e.g. EC_{10} or NOECs) value. In such cases the PNEC might be derived by using an assessment factor of 100 to the lowest L(E)C50 of the short-term tests".

Despite no toxicological effects in the short and long-term test were detected up to and exceeding the limit of water solubility, eMSCA agrees with the cautelative approach of the Registrant(s) to derive a tentative PNEC freshwater, but eMSCA considers that for chronic toxicity, the most sensitive species belongs to the trophic level of algae (NOEC$\geq$ 2.08 mg/L) and for acute toxicity the most sensitive seems *Daphnia*. As reported in table R10 -4, the calculation of the PNEC should be based on EC_{50}>0.1 mg/L (phenyl-C10, most water soluble single component) from 48-hr *Daphnia magna* study and AF = 100. Therefore eMSCA considers that the PNEC freshwater should be 0.001 mg/L.

PNEC marine water

eMSCA evaluated the PNEC marine water reported by the Registrant(s) and noted, in addition to the inconsistencies between the CSR and file IUCLID, that the chosen of assessment factor is not correct (AF=100). According to the same arguments reported above, eMSCA considers that three acute tests on three trophic levels and two chronic tests on two trophic levels (invertebrates and algae) are available and, therefore, according to chapter R10 the AF of 1000 must be taken into account : "*An assessment factor of 1000 applies also to the lowest of the two long-term results (e.g. EC_{10} or NOEC) covering two trophic levels (freshwater or saltwater algae and/or crustacean and/or fish) when such results (e.g. EC_{10} or NOEC) have not been generated for the species showing the lowest L(E)C_{50} of the short-term tests. This should not apply in cases where the acutely most sensitive species has an L(E)C_{50}-value lower than the lowest long term value. In such cases the PNEC might be derived by applying an assessment factor of 1000 to the lowest L(E)C_{50} of the short-term tests".*

In conclusion, taking into account of the arguments reported above for the PNEC freshwater calculation, eMSCA considers that the PNEC marine water should be 0.0001 mg/L.

PNEC sediment (freshwater and marine water)

In the CSR and in the IUCLID file the Registrant(s) reported PNECsediment(freshwater) of 16.5mg/Kg dw and $PNEC_{sediment}$ (marine water) of 1.65 mg/Kg dw, calculated with EPM method using NOEC=0.0075 mg/L. In addition to ECHA's considerations indicated in the CoRAP decision on the unreliability of this value and on the basis the above considerations for $PNEC_{freshwater}$ and $PNEC_{marinewater}$, eMSCA considers that for derivation of the correct $PNEC_{sediment}$ values with EPM method should be used EC_{50}>0.1 mg/L. However, eMSCA support the Registrant(s) conclusion that after evaluation of the terrestrial dataset, it becomes evident that indeed the EPM-derived $PNEC_{soil}$ showed to be a significant overestimation of the toxicity in the terrestrial compartment, when compared to the $PNEC_{soil}$ derived from the newly generated terrestrial toxicity studies (0.32 mg/kg soil dry weight to 3.7 mg/kg soil dry weight, respectively). In light of this, it can be assumed that the $PNEC_{sediment}$ derived by the EPM of 1.65 and 0.165 mg/kg soil dry weight for freshwater and marine water sediment, respectively, is also an overestimation.
According to ECHA Guidance R.10, $PNEC_{soil}$ was derived from the lowest NOEC result obtained from an OECD 208 terrestrial plants growth study and an assessment factor of 10.

eMSCA can support these soil hazard assessment conclusions, including the related PNEC derivation.

7.8.5. Conclusions for classification and labelling

HAB is not classified according to CLP. Short-term aquatic toxicity data are available for three trophic levels (fish, invertebrates and algae); long-term data are available for two trophic levels (invertebrates and algae). These studies show that HAB is generally considered to be non-toxic to aquatic organisms within the limits of water solubility.

7.8.6. Toxicokinetics

Not evaluated.

7.8.7. Acute toxicity and Corrosion / Irritation

Not evaluated.

7.8.8. Sensitisation

Not evaluated.

7.8.9. Repeated dose toxicity

Not evaluated.

7.8.10. Mutagenicity

Not evaluated.

7.8.11. Carcinogenicity

Not evaluated.

7.8.12. Toxicity to reproduction (effects on fertility and developmental toxicity)

Not evaluated.

7.8.13. Hazard assessment of physico-chemical properties

Not evaluated.

7.8.14. Selection of the critical DNEL(s) / DMEL(s) and / or qualitative / semi-quantitative descriptors for critical health effects

Not relevant for this evaluation.

7.8.15. Conclusions of the human health hazard assessment and related classification and labelling

Not evaluated.

7.9. Assessment of endocrine disrupting (ED) properties

Not evaluated.

7.10. PBT and VPVB assessment

1) Persistence

Based on evaluation of the biodegradation simulation studies in soil, conducted on a specific surrogate substance, **1,4-di-(2-decanyl)benzene**, considered representative of dialkyl benzenes, the major category of HAB, it can be concluded that the substance fulfills the criteria of Annex XIII. Therefore, the constituentis considered to be Persistent (P) and very Persistent (vP).

2) Bioaccumulation

The screening information available for the HAB indicate a potential of bioaccumulation (logK_{ow} values between 6.45 and 12.53 measured according to OECD 117). Registrant(s) provided one experimental study as a read-across reporting a BCF (aquatic species) of 35 L/kg ww, and BCF values estimated by QSARs for the 21 categories of the UVCB.
Based on the logk_{ow} values predicted by KOWWIN model for the selected individual structures representatives of the 21 categories, only the fraction (monoalkyl benzenes LAB, CAS 2719-61-1) has a logk_{ow} value of 7.87, whereas the other substances have logK_{ow} values exceeding 10 indicating high hydrophobicity. According to ECHA Guidance R.11 these predictions should be considered in qualitative terms.
Regarding the BCF values by QSAR, the results obtained are all very below 2000, including the cases with an estimated logk_{ow} value in the range of the training set (Category Representative monoalkyl benzenes LAB, Alkyl Alkylene Benzenes and Alkyl Phenyl Alkylene Benzenes).
Indeed, we cannot exclude that these substances might slowly bioaccumulate over time and eventually result in a high BCF value in long-term. In this respect, especially for so high logK_{ow} values (>10), the current experimental procedures do not allow to discriminate slow bioaccumulation processes. This might be an important issue to discuss in the next future, taking also into account that the PBT assessment in the guidelines would need to be revised accordingly.
Based on above argumentation eMSCA suspected slow bioaccumulation process. The available experimental methods are not suitable to identify slow but high bioaccumulation potential. As suggested by a commenting PBTEG member, as eMSCA for 1,1'-(isopropylidene)bis[3,5-dibromo-4-(2,3-dibromopropoxy)benzene] (TBBPA-DBPE, EC 244-617-5) case, the potential for slow bioaccumulation is addressed as a scientific issue: "*The high hydrophobicity of the substances (logK_{ow} > 10) raises a concern for slow bioaccumulation which however cannot be investigated further with existing validated methods. Based on the currently available PBT guidance (ECHA 2017) and the available data for TBBPA-DBPE, the eMSCA concludes that the B criterion for the substance is likely not fulfilled*".

3) Toxicity

According to the available information, HAB does not meet the T criteria based on human health classification.
HAB is not classified according to CLP. Short-term aquatic toxicity data are available for three trophic levels (fish, invertebrates and algae); long-term data are available for two trophic levels (invertebrates and algae). These studies show that HAB is generally considered to be non-toxic to aquatic organisms within the limits of water solubility.
Studies show that HAB is generally considered to be non-toxic to aquatic organisms at the limits of water solubility.
A 21-day chronic study with *Daphnia* exposed to LAB, the most water soluble component of HAB, still resulted in an EC_{50} of 0.012 mg/L and a NOEC of 0.0075 mg/L. While this latter value exceeds the T criteria, it was accomplished only by testing the most water soluble component of HAB and then further artificially enhancing solubility through use of acetone as a solvent. However, eMSCA notes several shortcomings that raise doubts about the relevance of this supporting study. Indeed there is a general lack of information on the test method ASTM E35.21 test guideline, Draft 5 (Proposed Standard Practice for Conducting Renewal Life Cycle Toxicity Tests with Daphnids) that is not equivalent to the standard OECD TG 211 and it is not among the methods indicated by the ECHA guidances. The ECHA

Guidelines R.7 states that NOEC values from long-term toxicity testing on Daphnia sp. can be used according to OECD 211 or equivalent test guidelines. Moreover the Key study based on the OECD TG 211 is performed using the most suitable WAF approach, as foreseen by OECD GD 23 for test material with low water solubility.
Moreover, eMSCA considers that data from standard toxicity tests, internationally harmonised test guidelines, are preferred. The results of the key study obtained from a test performed according to OECD Guideline 211 (Minderhout, Gallagher and Krueger, 2013) without the use of a solvent does not show chronic aquatic toxicity at the level of water solubility.
Due to the above uncertainties for the supporting study, eMSCA considers the registered HAB having not adverse long-term effects on Daphnia magna within water solubility range, based on outcome of the Key study (Minderhout, Gallagher and Krueger, 2013).
As a result, HAB is not considered to fulfil the T criterion.

4) Overall conclusion

Table 14 summarises the information available for constituents/categories of UVCB.

Table 14

Type	**CONCLUSION** **P**	**CONCLUSION B** EPISUITE v.4.11	**eMSCA Remarks**
1) dialkyl benzenes	**Confirmed P/vP**	BCF<2000*	**Confirmed P/vP by soil testing on: (1,4-di-(2-decanyl)benzene**
2) trialkyl benzenes	border-line (QSAR)	BCF<2000*	
3) alkyl dialkyl benzenes	/	BCF<2000*	
4) monoalkyl benzenes	/	BCF<2000	(questionable test **BCF =35** on **undecylbenzene** / 6742-54-7 229-806-2) Est. $logK_{ow}$ (7.87)
5) alkylindanes	border-line (QSAR)	BCF<2000*	
6) Alkyl Tetra-hydronaphthalenes	border-line (QSAR)	BCF<2000*	
7) Alkyl Alkylene Benzenes	/	BCF<2000	
8) Alkyl Octahydroanthracenes	border-line (QSAR)	BCF<2000*	
9) Alkylindenes	/	BCF<2000*	
10) Alkyl Dialkyl Dihydronaphthalenes	border-line (QSAR)	BCF<2000*	
11) Alkyl Tetraalkyl Dihydronaphthalenes	border-line (QSAR)	BCF<2000*	
12) Alkyl Alkylene Dihydronaphthalenes	border-line (QSAR)	BCF<2000*	
13) Alkylnaphthalenes	border-line (QSAR)	BCF<2000*	
14) Diphenyl Alkanes	Potentially P or vP (QSAR)	BCF<2000*	
15) Alkyl Diphenyl Alkanes	Potentially P or vP (QSAR)	BCF<2000*	

16) AlkylAcenaphthenes	border-line (QSAR)	BCF<2000*	
17) Phenyl Alkyl Tetra-hydronaphthalenes	Potentially P or vP (QSAR)	BCF<2000*	
18) Phenyl Alkyl Indanes	Potentially P or vP (QSAR)	BCF<2000*	
19) Alkyl Phenyl Alkylene Benzenes	Potentially P or vP (QSAR)	BCF<2000	
20) Alkyl Acenaphthylenes	border-line (QSAR)	BCF<2000*	
21) Alkyl Fluorenes	border-line (QSAR)	BCF<2000*	

*estimate **$logK_{ow}$ >10**, outside the training set's range (-1.37 to 11.26)

The registered substance results to be Persistent (P) and very Persistent (vP) based on the **1,4-di-(2-decanyl)benzene**, considered representative of **dialkyl benzenes group,** one of the most abundant Fraction of the UVCB. According to ECHA guidance R.11 this conclusion could be a first assessment tier of a UVCB substance if "fraction profiling approach" is applied for the PBT /vPvB concern.

eMSCA noted that the relevant constituent chosen for P assessment, **(1,4-di-(2-decanyl)benzene**), not necessarily represents a reasonable worst case for the whole PBT/vPvB assessment. However, due to the confirm of P/vP property for 1,4-di-(2-decanyl)benzene, Registrant(s) was definitely allowed to not provide any additional soil simulation test on other category representatives, identifying the whole UVCB fulfilling the P/vP criteria, as a consequence.

After the identification of the substance **1,4-di-(2-decanyl)benzene, representative of the group of dialkyl benzenes,** as P/VP, Registrant(s) did not addressed explicitly the B and T assessment according the "fraction-profyling approach", although QSARs estimation for aquatic BCF was provided for the 21 categories all resulting well below 2000.

eMSCA raises doubts on the applicability of the QSAR estimations for BCF values for the Fractions with $logK_{ow}$ outside the training set.
eMSCA consulted the PBT Expert Group on interpreting the data provided in order to properly conclude on PBT/vPvB concern.
Moreover eMSCA agrees that due to the very low water solubility and high $logK_{ow}$ values (almost all fractions with $logK_{ow}$ above 10), aquatic potential bioaccumulation is expected to be low.
eMSCA investigated which selected constituents/Fractions could be representative as regards PBT/vPvB concerns for the UVCB. For each group, eMSCA checked whether hypothetically it may contains constituents with combination of P, B (andT) properties of concern.

eMSCA acknowledges the lack of a clear indication of not-B only for the fraction of **Monoalkylbenzenes**, but no indication of P is present for this fraction. On the other hand, the group of **dialkyl benzenes** is the only fraction confirmed as P, based on an OECD 307 study for the representative substance 1,4-di(2-decanyl)benzene, that however, is supposed not potential B according to Annex XIII criteria (very high hydrophobicity and QSAR estimation).

Moreover at the eMSCA did not considered feasible the possibility to require additional experimental tests for each constituent/category to check further whether the complex UVCB hypothetically may contain constituents with combinations of P and B properties of concern.

In conclusion, according to the current knowledge, considering all the data available, it seems unlikely to identify a combination of P, B (and T) properties in one single constituent/fraction, among nearly 1000 estimated constituents for the registered UVCB. A whole substance approach seems more appropriate, using the WoE of all the data available

7.11. Exposure assessment

7.11.1. Human health

7.11.1.1. Worker

For workers, eMSCA agrees with the approach followed by the Registrant(s) in performing the exposure and risk assessment for human health.

7.11.1.2. Consumer

For consumers, eMSCA agrees with the approach followed by the Registrant(s) in performing the exposure and risk assessment for human health.

7.11.2. Environment

In order to clarify the possible impact on the environment, pursuant to Article 46(1) of the REACH Regulation, the Registrant(s) was requested to submit additional information related to the environmental exposure assessment and risk characterization to conclude on the initial concerns (wide dispersive use/consumer use/exposure and high aggregated tonnage) and on the identified additional concern (potential risk for soil compartment). In particular, the Registrant(s) was requested to provide a detailed description of adopted Operational conditions (OCs) and Risk management measures (RMMs) for all the relevant ESs, including a justification for the discrepancies between the Emission Days reported in certain ESs and those associated with some specific Specific Environmental Release Categories (SPERCs) as well as for not adopting the safety factor of 4 in the calculation of regional tonnage and daily widespread use of the substance for the ESs related to wide dispersive uses. Also, the Registrant(s) was requested to develop distinct exposure scenarios for not similar uses, giving to the ES an appropriate short title and a brief general description of the use(s) covered, selecting the relevant worst-case ERC for the risk characterization, in cases where more than one ERC was assigned. Moreover, the Registrant(s) was requested to perform an environmental exposure assessment and risk characterisation of the uses related PC28, and PC39. Lastly, the Registrant(s) was requested to properly characterize the risk for soil compartment and thus to refine the quantitative exposure assessment and to update accordingly the risk characterization.

Taking into account the uses of the substance the Registrant(s) provided all the requested elements for a refined assessment of the environmental exposure. Although not described in detail, the OCs and the RMMs adopted for all the exposure scenarios have been schematically indicated by the Registrant(s) and are in agreement with the identified ERC or SPERC categories. Also, in the contributing scenarios controlling environmental exposure, the Registrant(s) applied the default values for release factors taken from ERCs, or refinements according to available SPERCs (ATIEL, ESVOC and CEPE). For some uses, mainly for professional workers, Registrant(s) claim that the assigned release factors were reviewed and agreed upon by a broad group of knowledgeable specialists within sector organizations. For some scenarios, the approach used to assign the release values is largely qualitative in nature and takes advantage of the sector knowledge and professional judgement of individuals within the expert group responsible for creating this SpERC factsheet. The Registrant(s) identifies, appropriately, all uses by professional workers, consumer and service life scenarios as being wide dispersive (ESs 16-39). Related to the estimation of the daily tonnages, the eMSCA notes that the Registrant(s) applies the safety factor of 4 only in the ES29 ‘professional end-use in agrochemicals’. ECHA guidance R16

clearly indicate that this safety factor should be applied to all the wide dispersive uses to take into account geographical or temporal peaks in the use of a substance. However Registrant(s) can overwrite this value, if they have sufficient information to demonstrate that the use of the substance is evenly distributed in space and time throughout the region. In this case, this assumption could be considered justified based on the above mentioned refinements with the SPERCs used by Registrant(s).

In conclusion, despite some uncertainties, eMSCA considers that the level of exposure for the different environmental compartments is adequate.

7.11.2.1. Aquatic compartment (incl. sediment)

As stated in the supporting document provided by the Registrant(s), all reported RCR values in the exposure scenarios for manufacturing, industrial and consumer use are less than 1 and the risk is considered to be controlled in each aquatic environment.
The eMSCA notes that the Registrant(s) correctly applies the standard RFs from the ERC or SPERC categories in the assessment of aquatic compartment. However, the eMSCA deems questionable the Registrant(s)' assumption according to which the safety factor of 4 is only applied in the ES29 to estimate the daily tonnage of the substance and not in all the identified widespread uses. ECHA guidance R16 clearly indicate that this safety factor should be applied to all the wide dispersive uses to take into account geographical or temporal peaks in the use of a substance. However eMSCA notes that Registrant(s) can overwrite this value, if they have sufficient information to demonstrate that the use of the substance is evenly distributed in space and time throughout the region. Despite some uncertainties, however, eMSCA considers that the level of exposure for the aquatic compartment is acceptable.

7.11.2.2. Terrestrial compartment

The substance is neither directly nor indirectly released to soil due to adequate technical and organizational measures and therefore releases to this compartment are considered negligible. The sludge generated from wastewater treatment is not applied to agricultural soil.
In conclusion, all reported RCR values calculated in the exposure scenarios are less than 1 and the risk is considered to be controlled in this environmental compartment.
The eMSCA notes that the Registrant(s) correctly applies the standard RFs from the ERC or SPERC categories in the exposure assessment for the substance uses in the terrestrial compartment. However, due to the presence of uncertainties in the exposure assessment provided by the Registrant(s), the eMSCA considers that the calculated local PEC values for the terrestrial compartment might be underestimated. Despite some of inconsistencies, however, eMSCA considers that the level of exposure for terrestrial compartment is acceptable.

7.11.2.3. Atmospheric compartment

Although for various scenarios of manufacturing and industrial use, the release values are very high, also higher than other compartments, the Registrant(s) have adopted appropriate RMMs and OC such that the risk for atmospheric compartment is considered to be controlled.
The eMSCA notes that the Registrant(s) correctly applies the standard RFs from the ERC or SPERC categories in the exposure assessment for the substance uses. Despite some of uncertainties, however, eMSCA considers that the exposure estimate for atmospheric compartment is acceptable.

7.11.3. Combined exposure assessment

Registrant(s) provided the total releases to the environment as the sum of the releases to the environments from all exposure scenarios addressed.

Registrant(s) provided adequately also the regional predicted environmental concentration ($PEC_{regional}$), the Predicted exposure concentrations and risks for the environment and man via the environment due to all widespread uses, and the related risk characterisation ratios. The exposure estimates have been obtained with EUSES 2.1.2.

7.12. Risk characterisation

For the human health, the overall risk characterization is acceptable and the risks can be considered under control.
Environment
In response to the Substance Evaluation decision, the Registrant(s) provided a refined risk assessment for all compartments, particularly for the terrestrial one. The eMSCA considers that the risk is adequately controlled in all the environmental compartments, since all the respective RCR values are fairly below 1.

7.13. References

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Phillips C.R. *et al*., 2001) Linear Alkylbenzenes in muscle tissues of White Croaker near a large Ocean Outfall in Southern California, Usa, Environmental Toxicology and Chemistry, Vol. 20, No. 2, pp. 231–238.

7.14. Abbreviations

AF	Assessment Factor
BCF	Bioconcentration Factor
BCFBAF	Bioconcentration Factor-Bioaccumulation Factor
CLP	Classification, Labelling and Packaging
CoRAP	Community Rolling Action Plan
CSA	Chemical Safety Assessment
CSR	Chemical Safety Report
EbC_{50}	Concentration of test substance which results in a 50 percent reduction in biomass growth(EbC_{50}) relative to the control within 72hrs exposure
EC_{10}	Concentration estimated to immobilise 10 per cent of the daphnids within a stated exposure period
EC_{50}	Concentration estimated to immobilise 50 per cent of the daphnids within a stated exposure period. If another definition is used, this must be reported, together with its reference.
eMSCA	evalutating Member State Competent Authority
ErC_{50}	Concentration of test substance which results in a 50 percent reduction in growth rate (ErC_{50}) relative to the control within 72hrs exposure
EPM	Equilibrium Partitioning Method
ERCs	Environmental Release Categories
ES	Exposure Scenario
GLP	Good Laboratory Practice
HAB	Benzene, mono-C10-13-alkyl derives., distillation residues
LAB	Linear alkylbenzene
MW	Molecular Weight
NER	Non-Extractable Residues
NOEC	No Observed Effect Concentration

OCs	Operational Conditions
PAH	Polycyclic Aromatic Hydrocarbon
PBT/vPvB	Persistent, Bioaccumulative and Toxic/very Persistent and very Bio-accumulative
PBT EG	PBT Expert Group
PC	Product Category
PEC	Predicted Environmental Concentration
PNEC	Predicted No-Effect Concentration
QSAR	Quantitative Structure-Activity Relationship
RAA	Read Across Assessment
RCR	Risk Characterisation Ratio
RFs	Release Factors
RMMs	Risk Management Measures
SPERC	Specific Environmental Release Categories
TG	Technical Guidance
WAF	Water-Accommodated Fraction