SUBSTANCE EVALUATION CONCLUSION

as required by REACH Article 48

and

EVALUATION REPORT

for

Diisotridecyl adipate (DITA)

EC No 247-660-8

CAS No 26401-35-4

Evaluating Member State(s): Spain

Dated: 20 May 2018

Evaluating Member State Competent Authority

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Year of evaluation in CoRAP: 2013

Before concluding the substance evaluation a Decision to request further information was issued on: 2 September 2015

Further information on registered substances here:

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

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

Diisotridecyl adipate was originally selected for substance evaluation in order to clarify concerns about:

- suspected PBT properties
- lack of exposure assessment,
- wide dispersive use, and
- high (aggregated) tonnage.

During the evaluation also other concerns were identified. The additional concerns were:

- environmental classification
- high risk characterization ratios (RCRs) for the environment

2. OVERVIEW OF OTHER PROCESSES / EU LEGISLATION

No other ongoing processes/ EU legislation relevant for the substance evaluation.

3. CONCLUSION OF SUBSTANCE EVALUATION

Table 1.

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

4. FOLLOW-UP AT EU LEVEL

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

4.1.1. Harmonised Classification and Labelling

Diisotridecyl adipate has currently no harmonised classification in Annex VI of CLP Regulation (Regulation (EC) 1272/2008) and the registrants have not self-classified the substance for any endpoints. No classifications are notified in the C&L inventory either.

However, the eMSCA concludes as a result of the substance evaluation that, based on the outcome of the recent Daphnia magna reproduction study (OECD 211), diisotridecyl adipate should be classified as Aquatic Chronic 1 (M-factor=1).

The eMSCA advises the registrants to revise their self-classification of the substance and implement appropriate risk management measures. The need for harmonised classification and labelling is not currently considered as a priority if the companies placing the substance in the market in the EU ensure that the substance is appropriately self-classified.

4.1.2. Identification as a substance of very high concern, SVHC (first step towards authorisation)

Not applicable.

4.1.3. Restriction

Not applicable.

4.1.4. Other EU-wide regulatory risk management measures

Not applicable.

5. CURRENTLY NO FOLLOW-UP FORESEEN AT EU LEVEL

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

Based on the available registration information, QSAR modelling performed by the eMSCA and additional information provided by the registrant on the composition of the substance, the eMSCA concludes that the initial concern on potential PBT/vPvB properties of diisotridecyl adipate can be removed. Therefore no regulatory risk management follow up action is needed with regards to PBT/vPvB properties at this time.

No concerns on the RCRs of the relevant environmental compartments remain after the refinement of the exposure assessment.

5.2. Other actions

Not applicable.

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

Table 2.

FOLLOW-UP		
Follow-up action	**Date for intention**	**Actor**
CLP Annex VI dossier for environmental classification and labelling in case self-classification not revised by registrants	*Not available*	A member state competent authority

The need for harmonised classification and labelling is not currently considered as a priority if the companies placing the substance in the market in the EU self-classify appropriately the substance and implement the appropriate risk management measures for handling the substance.

Part B. Substance evaluation

7. EVALUATION REPORT

7.1. Overview of the substance evaluation performed

Diisotridecyl adipate was originally selected for substance evaluation in order to clarify concerns about:

- suspected PBT properties
- lack of exposure assessment,
- wide dispersive use, and
- high (aggregated) tonnage.

During the evaluation also other concerns were identified. The additional concerns were:

- environmental classification
- high RCRs for the environment

Table 3.

EVALUATED ENDPOINTS	
Endpoint evaluated	**Outcome/conclusion**
Suspected PBT properties	Concern not substantiated. No further action.
Lack of exposure assessment	Concern not substantiated. Exposure assessed. No further action.
High RCRs for the environment	Concern not substantiated. No further action.
Environmental classification	Need for environmental classification confirmed.

7.2. Procedure

Diisotridecyl adipate (DITA) was included in the Community Rolling Action Plan (CoRAP) list to be evaluated by the Spanish CA in 2013 due to initial concerns on potential PBT/vPvB properties, lack of exposure assessment, high (aggregated) tonnage and wide dispersive use.

On 20 March 2013 the updated CoRAP list was published on the ECHA website and the evaluation was officially started. The scope of the evaluation was the environmental data. From the human health endpoints only the data relevant for the PBT concern was briefly reviewed.

During the evaluation the eMSCA identified additional concerns related to potential environmental classification and high risk characterisation ratios for the environment.

The evaluation was based on the registration information and other additional information provided by the registrants during the evaluation, e.g. a new OECD 301F study voluntarily performed by the registrants in May 2014.

The environmental exposure assessment was carried out using the information presented by the registrants and the default exposure values according to the CHESAR/EUSES models.

The eMSCA considered that further information was required to clarify the concerns on potential environmental classification and lack of exposure assessment. Therefore, it prepared a draft decision pursuant to Article 46(1) of the REACH Regulation to request further information. It submitted the draft decision to ECHA on 19 March 2014.

The Registrant(s), the Competent Authorities of other Member States and ECHA were invited to provide comments and proposals for amendments to the draft decision in accordance with the procedure described in the REACH Regulation. A detailed description of the commenting phase, including the dates, can be found in the Substance Evaluation Decision of the substance. A unanimous agreement of the Member State Committee on the draft decision as amended in the meeting was reached on 5 February 2015.

On 2 September 2015 the Substance Evaluation Decision requesting a Daphnia magna reproduction test (OECD 211) and information to refine the exposure assessment was sent to the Registrant(s). The deadline to provide the requested information was set to 9 September 2016. The requested information was uploaded by registrants in an updated registration dossier on 9 September 2016.The provided information was reviewed by the eMSCA.

As DITA is an UVCB substance consisting of complex isomers of the isotridecyl alcohol chain with more than 50 possible isomers, the PBT assessment has to take into account all isomers present at or above a concentration of 0.1% (w/w). Additional clarifications on the substance composition provided by the registrants in July 2017 removed the concern on the presence of potential persistent isomers in the substance.

Based on the outcome of the Daphnia magna reproduction study, the eMSCA concluded that the substance requires a classification of Aquatic Chronic 1 and that the registrants should update the self-classification of the substance and implement appropriate risk management measures. The need for harmonised classification and labelling is not currently considered as a priority if the companies placing the substance in the market in the EU ensure that the substance is appropriately self-classified.

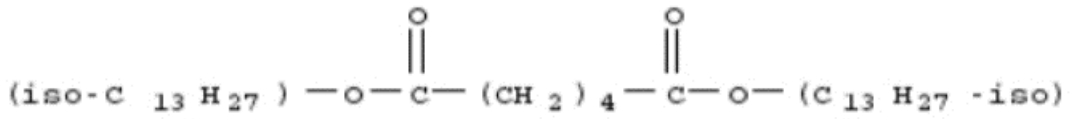
7.3. Identity of the substance

Table 4.

SUBSTANCE IDENTITY	
Public name:	Diisotridecyl adipate
EC number:	247-660-8
CAS number:	26401-35-4
Index number in Annex VI of the CLP Regulation:	-
Molecular formula:	C32H62O4
Molecular weight range:	510.8323
Synonyms:	DITA DTDA Bis(11-methyldodecyl) adipate Bis(11-methyldodecyl) hexanedioate Hexanedioic acid, di(C11-C14-iso, C13 rich iso alkyl) esters Hexanedioic acid, diisotridecyl ester Ketjenlube 15 Cereplas DTDA GLYPLAST DTDA Hedilub-LB/508 Linplast 13 XA Paryol DTDA Reproxal 13 XA

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

Structural formula:



UVCB substance

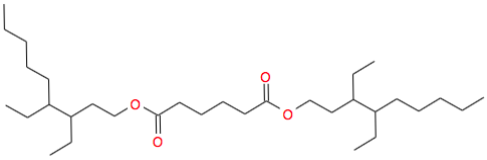
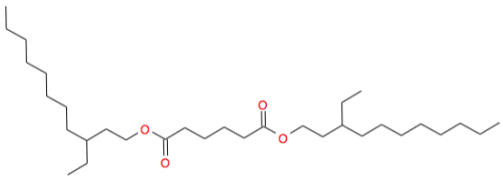
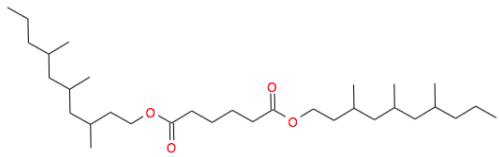
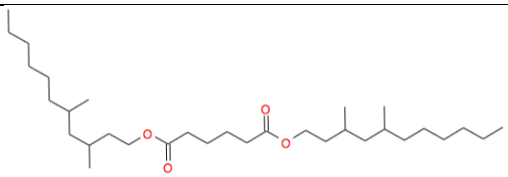
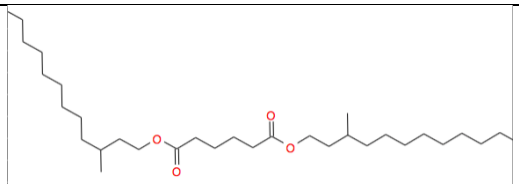
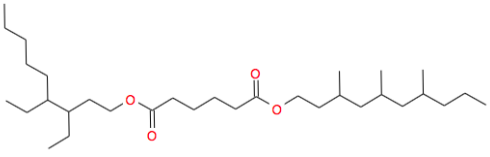
Diisotridecyl adipate is an UVCB substance. The constituents are diesters of a dicarboxylic acid consisting of adipic acid (C6) and isotridecyl alcohols with a branched carbon chain (C13). The constituents differ in the branching of the diisotridecyl carbon chain. Several different isomers (> 50) are possible.

Since according to Annex XIII of REACH, the PBT assessment has to take into account all constituents present at a concentration of ≥ 0.1 % (w/w) the eMSCA has performed QSAR predictions for example isomers representing the most common type of isomers (isomers 1-6 in table 5) as well as for theoretical worst-case isomers (isomers 7 and 8 in table 5) according to the information provided by the registrant. It is noted that the theoretical worst case isomers contain one or two quaternary carbons (quat-C) which are usually expected to be relatively poorly biodegraded. However, based on the available

information on the starting materials and manufacturing process of the substance as well as on the available analytical data, provided to the eMSCA by the registrants, the presence of constituents with quaternary carbons seems unlikely. Nevertheless, as DITA is a UVCB substance, the composition of isomers may vary in different batches and between different manufacturers. Therefore, these type of isomers were included as theoretical worst case constituents in the QSAR analyses in order to assess the PBT status of all theoretically possible isomers. The worst case isomers contain only one or two quaternary carbons as the presence of more quaternary carbons was considered very unlikely. The position of the quaternary carbons were chosen randomly as the QSAR models performed do not differentiate between the different positions of quat-C, e.g. between terminal and non-terminal quat-C.

Further information on the constituents and manufacturing process is considered confidential and it is included in the confidential annex of this document.

Table 5

REPRESENTATIVE ISOMERS USED IN THE QSAR MODELS			
No.	Sidechains	Smiles	Structure
1	Two 3,4-diethlynonanols	CCCCCC(CC)C(CC)COC(=O)CCCCC(=O)OCCC(CC)C(CC)CCCCC	
2	Two 3-ethylundecanols	CCCCCCCCC(CC)COC(=O)CCCCC(=O)OCCC(CC)CCCCCCCC	
3	Two 3,5,7-trimethyldecanols	CCCC(C)CC(C)CC(C)CCOC(=O)CCCCC(=O)OCCC(C)CC(C)CC(C)CCC	
4	Two 3,5-dimethylundecanols	CCCCCCC(C)CC(C)COC(=O)CCCCC(=O)OCCC(C)CC(C)CCCCCC	
5	Two 3-methyldodecanols	CCCCCCCCCC(C)COC(=O)CCCCC(=O)OCCC(C)CCCCCCCCC	
6	One 3,5,7-trimethyldecanol and one 3,4-diethylnonanol	CCCCCC(CC)C(CC)COC(=O)CCCCC(=O)OCCC(C)CC(C)CC(C)CCC	

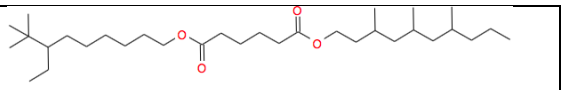
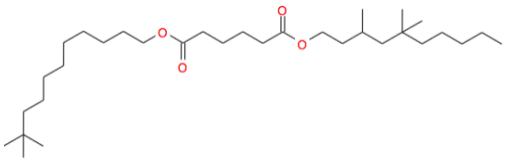
7	One 3,5,7-trimethyldecanol and one 7-ethyl, 8,8-dimethylnonanol	CC(C)(C)C(CC)CCCCCCOC(=O)CCCCC(=O)OCCC(C)CC(C)CC(C)CCC	
8	One 3,5,5-trimethyldecanol and one 10,10-dimethylundecanol	CC(C)(C)CCCCCCCCCOC(=O)CCCCC(=O)OCCC(C)CC(C)(C)CCCCC	

Table 6

Constituent **Constituents**	**Typical concentration**	**Concentration range**	**Remarks**
Different isomers of diisotridecyl adipate EC 247-660-8	*	*	*

* confidential information

Similar substances

Information on the structurally similar substances in the following tables (Tables 7-9) is used as supporting information in some endpoints, e.g. in bioaccumulation and aquatic toxicity. Diisotridecyl adipate, bis (2- ethylhexyl) adipate and diisooctyl adipate are all dialkylesters of the same dicarboxyl acid, adipic acid (1,6- hexanedioic acid). They differ in the length (C8 vs. C13) and branching of the alkyl groups. Diisotridecyl adipate and diisotridecyl dodecanedioate are both UVCB substances that have the same alcohol component (C13) but a different dicarboxylic acid (C6 vs C12).

Table 7. Bis (2- ethylhexyl) adipate (DEHA)

SIMILAR SUBSTANCE	
Public name:	Bis (2- ethylhexyl) adipate
EC number:	203-090-1
CAS number:	103-23-1
Index number in Annex VI of the CLP Regulation:	-
Molecular formula:	C22H42O4
Molecular weight range:	370.57
Synonyms:	DEHA Di(2-ethylhexyl) adipate

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

Structural formula:

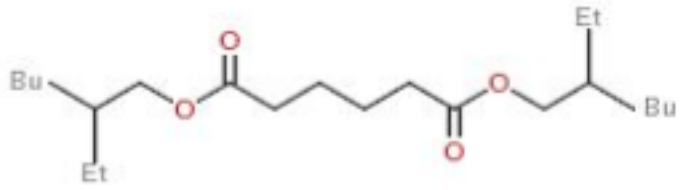


Table 8. Diisooctyl adipate

SIMILAR SUBSTANCE	
Public name:	Diisooctyl adipate
EC number:	215-553-5
CAS number:	1330-86-5
Index number in Annex VI of the CLP Regulation:	-
Molecular formula:	C22H42O4
Molecular weight range:	370.57
Synonyms:	

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

Structural formula:

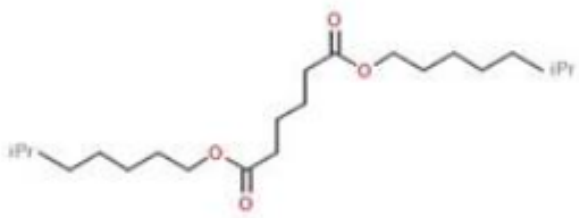
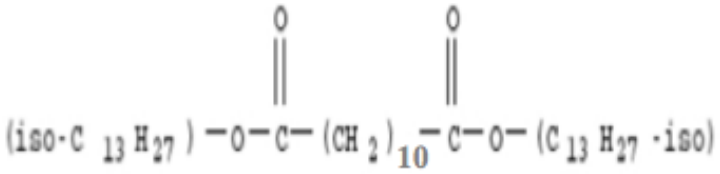


Table 9. Diisotridecyl dodecanedioate

SIMILAR SUBSTANCE	
Public name:	Diisotridecyl dodecanedioate
EC number:	283-822-4
CAS number:	84731-63-5
Index number in Annex VI of the CLP Regulation:	-
Molecular formula:	C38H74O4
Molecular weight range:	595
Synonyms:	

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

Structural formula:



7.4. Physico-chemical properties

Table 10.

OVERVIEW OF PHYSICOCHEMICAL PROPERTIES	
Property	**Value**
Physical state at 20°C and 101.3 kPa	Clear and yellowy organic liquid
Vapour pressure	The vapour pressure of DITA was determined to be 0.0054Pa at 25°C
Melting point	-62ºC
Boiling point	321ºC
Water solubility	A water solubility of 0.7µg/L at 20°C in deionised water measured using OECD 105 column elution method is reported. In addition to the determination of water solubility in deionized water, as laid out in the OECD 105 guideline, side experiments were performed to assess the solubility of diisotridecyl adipate in ecotoxicological test media using the column elution method (purified test water and ISO standard medium). The concentrations measured in these medias ranged from 12 µg/L to 19.7µg/L. However, the variability of the measured concentrations among the individual replicates was higher than in the deionized water. Deviations from the standard guideline (such as loaded material, loading rate and flow rate) has been observed. The presence of undissolved test material or micelle formation is not visually observed, although it cannot be excluded. In the literature a water solubility of < 0,001 mg DITA /L is described. EPISuite QSAR models predict water solubility in the range of 4.6×10^{-9} – 5.1×10^{-5} mg/L for different isomers of DITA (see table 11). These values support the results of the OECD 105 study using column elution method.. The measured value of 1.12 mg/L (Registration dossier, study report 2010) has been determined using the flask method. In the guideline (R7.A) this method is recommended for substances with higher water solubility (> 10 mg/L). Therefore this method is not appropriate for determination of the water solubility of DITA. Two other existing experimental results in the registration dossier, also performed in 2010, are considered as limit tests up to the detection limits of the used analytical method.

Partition coefficient n-octanol/water (Log Kow)	The partition coefficients of different representative isomers of the substance were determined by EPISuite KOWWIN calculation to be in the range of 12.77-13.03 (see table 11).
Flammability	waived
Explosive properties	waived
Oxidising properties	waived
Granulometry	waived
Stability in organic solvents and identity of relevant degradation products	waived
Dissociation constant	waived

Table 11.

PREDICTED LOG KOW AND WATER SOLUBILITY OF THE REPRESENTATIVE ISOMERS		
Isomer*	Log Kow (KOWWIN v1.68)	Water solubility (mg/L) (WSKOW v1.42/ WATERNT v1.01)
1	12.88	6.114e-009 / 5.1085e-007
2	13.03	4.579e-009 / 5.1085e-007
3	12.73	8.163e-009 / 5.1085e-007
4	12.88	6.114e-009 / 5.1085e-007
5	13.03	4.579e-009 / 5.1085e-007
6	12.81	7.064e-009 / 5.1085e-007
7	12.77	7.607e-009 / 5.1085e-007
8	12.88	6.134e-009 / 5.1085e-007

* See Table 5 for further information on the representative isomers.

7.5. Manufacture and uses

7.5.1. Quantities

As it has been indicated, this UVCB substance can contain several different multibranched isomers. Based on the knowledge of the starting materials and according to the expert judgement provided to the eMSCA by the registrant, predominantly structures like ethylundecanol and diethlynonanol but also trimethyldecanol, dimethylundecanol, and methyldodecanol are expected in the sidechains of DITA. Based on the analytical data, on average two branches per isotridecanol are expected with branching starting in the C2 position.

In order to exclude the presence of potential persistent constituents of DITA (i.e. isomers with quaternary carbons) some non-confidential information on the production steps is included below, based on theoretical considerations.

According to registrants´ information, isotridecanol (ITD) is used as starting material in the manufacture of DITA. The production of ITD is a two step process:

- In the first step 1-butene is oligomerized giving dibutene, tributene and higher oligomers. These oligomers are separated via distillation.
- In the second step the tributene is converted in an oxo process into the corresponding alcohol.

First step: Oligomerisation

In this process the 1-butene is treated with a solid heterogeneous catalyst.
The primary step is the formation of a dimer (R_1 and R_2 are CH_2CH_3).

$$R_1\text{-}CH{=}CH_2 + R_2\text{-}CH{=}CH_2 \longrightarrow R_1\text{-}CH_2\text{-}CH_2\text{-}CR_2{=}CH_2 \text{ or } HCH_2\text{-}CHR_1\text{-}CR_2{=}CH_2 \text{ or}$$
$$R_1\text{-}CH_2\text{-}CH_2\text{-}CH{=}CHR_2 \text{ or } HCH_2\text{-}CHR_1\text{-}CH{=}CHR_2$$

In this primary step already at least four different isomers will be built. But none of these isomers contains quaternary carbons.

In the secondary step the dimer reacts with an additional 1-butene resulting in a lot of different isomers.

And even if the double bond would "move" along the C-chain of the molecule all final isomers will have comparable structures to the four mentioned above except that the R_1 and R_2 are not only ethyl groups but any linear or mono-branched alkyl group. Therefore the presence of any quaternary carbon or any t-butyl-group can be excluded for the tributene.

To confirm this theoretical approach, registrants run a Distortionless Enhancement of Polarisation Transfer – Carbon Nuclear Magnetic Resonance (DEPT CNMR) with tributene. Not any quaternary carbon could be detected. CNMR analytics of the hydrogenated tributene shows that on average 2.0 tertiary C-atoms per molecule are present.

Second step: Building of alcohols

The olefins are treated in an oxo process with CO and H_2 in the presence of a cobalt or rhodium complex. Usually $HCo(P_2)(CO)_2$ or $HRh(P_2)(CO)_2$; (P_2) is normally a chelating ligand containing 2 phosphine groups; typical examples are $Ph_2P\text{-}CH_2\text{-}CH_2\text{-}PPh_2$ and derivatives thereof) acting as a catalyst.

First a corresponding aldehyde is produced which is further hydrogenated to the corresponding primary alcohol. Depending on the used catalyst the double bond might "move" along the C-chain of the olefin prior to the formation of the aldehyde.

Due to the big catalyst molecule the attack of the CO to the double bond is sterically hindered and therefore the terminal C-atom of a terminal double bond is preferred. In the double bond located inside the C-chain that carbon atom is attached that has less steric hindrance meaning less alkyl groups. Therefore also in this production step, the formation of quaternary carbons is highly unlikely.

In order to confirm this theoretical approach, analytical confirmation was prepared. The two CNMR spectra of isotridecanol DEPT and JMSE[2] molecular editor clearly show that no quaternary carbons (Cq) are present. The conclusion of the report summarizes: "The 13C NMR spectrum of the sample shows a complex mixture of isomers. Therefore, just a DEPT135 spectrum is not suitable to check for quaternary carbons in the mixture. An additional JMSE was measured, which allows to detect Cq. The residual signals were compared with the DEPT135. Signals in the JSME without equivalent in the DEPT135. No Cq could be detected, with the exception of the strong CDCl3 signal of the NMR solvent at about 77 ppm."

The analytical report provided indicated that no quaternary carbon signal was present.

Table 12.

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

DITA has widespread uses as it is used in lubricants and greases by consumers and professional workers and it is present in articles. The substance is also used in formulation and/or re-packing and at industrial sites.

Table 13.

USES	Use(s)
Uses as intermediate	-
Formulation	Formulation of polymers, lubricants, lubricant additives, greases and metal working fluids. Formulation of laboratory chemicals
Uses at industrial sites	Use in lubricants and greases in open processes and in vehicles and machinery. Use in polymer processing and in plastisol.
Uses by professional workers	Use in lubricants and greases in open processes and in vehicles and machinery. Indoor and outdoor use.
Consumer Uses	Use in polymers, lubricants and greases in vehicles and machinery. Indoor and outdoor use.
Article service life	Plastic articles (e.g. food packaging and storage, toys, mobile phones).

[2] http://peter-ertl.com/jsme/

7.6. Classification and Labelling

7.6.1. Harmonised Classification (Annex VI of CLP)

No harmonised classification in Annex VI of CLP Regulation (Regulation (EC) 1272/2008).

7.6.2. Self-classification

- In the registration(s)*:*

No classification.

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

No classification.

7.7. Environmental fate properties

7.7.1. Degradation

7.7.1.1. **Hydrolysis**

The registration dossier includes HYDROWIN v 2.00 (EPI Suite v4.00) predictions for the hydrolysis rate and half-life of diisotridecyl adipate. The total basic (pH 8) hydrolysis rate constant for DITA at 25°C was calculated to be 0.04737 L/(mol*s). The half-lives were estimated to be 169 days at pH 8 and 4.6 years at pH 7.

7.7.1.2. **Phototransformation/photolysis**

No relevant information available

7.7.1.3. **Biodegradation**

7.7.1.3.1. Biodegradation in water

Estimated data

Since there is no experimental data on the degradation of individual isomers of DITA, EPISuite BIOWIN v4.10 models were performed for representative isomers of DITA (see table 5 for further information on the representative constituents) in order to carry out a screening assessment of persistence for possible constituents. According to the REACH Guidance on Information Requirements and Chemical Safety Assessment, Chapter R.11: PBT/vPvB assessment, Version 3.0, June 2017, the following outcome indicate that a substance may be persistent: BIOWIN 2 <0.5 and BIOWIN 3 <2.2 or BIOWIN 6 <0.5 and BIOWIN 3 <2.2. However, borderline cases should be carefully examined, e.g. when the estimate of the BIOWIN 3 gives a result in the range 2.25 to 2.75. The results of the QSAR models are shown in Table 14.

The BIOWIN 2 model predicts that all the representative isomers are readily biodegradable. In contrast, according to the BIOWIN 6 predictions, the isomer 3 is not readily biodegradable and the results of the isomers 6 and 7 are very close to the screening cut off value. The BIOWIN 3 result of isomer 7 fulfils the screening criterion for

persistence and the results of isomers 3,6 and 8 are borderline cases. In summary, the isomers 3, 6-8 are borderline cases for meeting the screening criteria.

The contradicting results of the BIOWIN 2 and 6 models can be explained by the fragments and their coefficients included in the two models. In the BIOWIN 2 model, only ester groups, quaternary carbons and linear C4 terminal chain fragments are included, whereas in the BIOWIN 6 model also methyl, secondary (-CH2-) and tertiary carbon (–CH-) fragments are included. In this model, tertiary carbons have a negative coefficient and hence, isomers with more tertiary carbons are predicted to be degraded slower. Another difference between the two models is that in the BIOWIN 2 model quaternary carbons have a negative coefficient while in the BIOWIN 6 model they have a positive coefficient. Hence, the BIOWIN 6 model could be considered to be more reliable than BIOWIN 2 for the isomers of DITA as it takes into account more fragments.

The positive coefficient of quaternary carbons used in BIOWIN 6 adds some uncertainty to the predictions of this type of structures since they are often considered to be poorly degradable. Some uncertainty arises also from the fact that the BIOWIN models do not differentiate between quaternary carbons at terminal and non-terminal positions. According to Pitter and Chudoba (1990), complex branching, particularly the presence of quaternary carbon atoms, could impede the normal biodegradative pathway of β-oxidation and further metabolism is dependent on less common pathways. Compounds with a tertiary/quaternary carbon atom can be stable due to steric effects. In particular, terminal quaternary carbons are known to often inhibit biodegradation.

In conclusion, based on the BIOWIN models, which are not fully reliable for the isomers of DITA, most of the isomers representing the most common structures of the substance are expected to be readily biodegradable. The isomers with higher degree of branching (at least 5 branches in total in the two side chains) as well as isomers with quaternary carbons could be potentially persistent. However, as indicated above in the section 7.5.1, it is unlikely that DITA contains isomers with quaternary carbons.

Table 14.

BIOWIN QSAR PREDICTIONS FOR REPRESENTATIVE ISOMERS OF DITA

Isomer*	BIOWIN 2	BIOWIN 3	BIOWIN 6
1	0.9995	2.9474	0.7267
2	0.9995	2.9474	0.9457
3	0.9804	2.3507	0.2889
4	0.9995	2.9474	0.7267
5	0.9995	2.9474	0.9457
6	0.9969	2.6490	0.5096
7	0.8994	2.1386	0.5317
8	0.9098	2.2248	0.8904

* See Table 5 for further information on the representative isomers.

It is also noted that the results of BIOWIN 4 model were between 3 and 4 (i.e. days or weeks) for all representative isomers, which suggests that primary degradation may occur relatively rapidly. Based on the EAWAG Biodegradation pathway predictions, the

most likely first transformation steps for all the isomers are the cleavage of the ester bonds leading to the formation of adipic acid and isotridecyl alcohols (see below Figure 1). Based on the available information[3], adipic acid is readily biodegradable as well as isotridecyl alcohol as a whole substance. Some differences in the degradation rate of different isomers of the isotridecyl alcohol could be possible but based on the very rapid and complete degradation observed for the whole substance in a ready biodegradation test reported in the registration dossier of the substance (66 % after 11 days and 98 % after 28 days based on O_2 consumption), it can be expected that none of the isomers is persistent.

[3] Information in the registration dossiers of EC 204-673-3 and EC 248-469-2

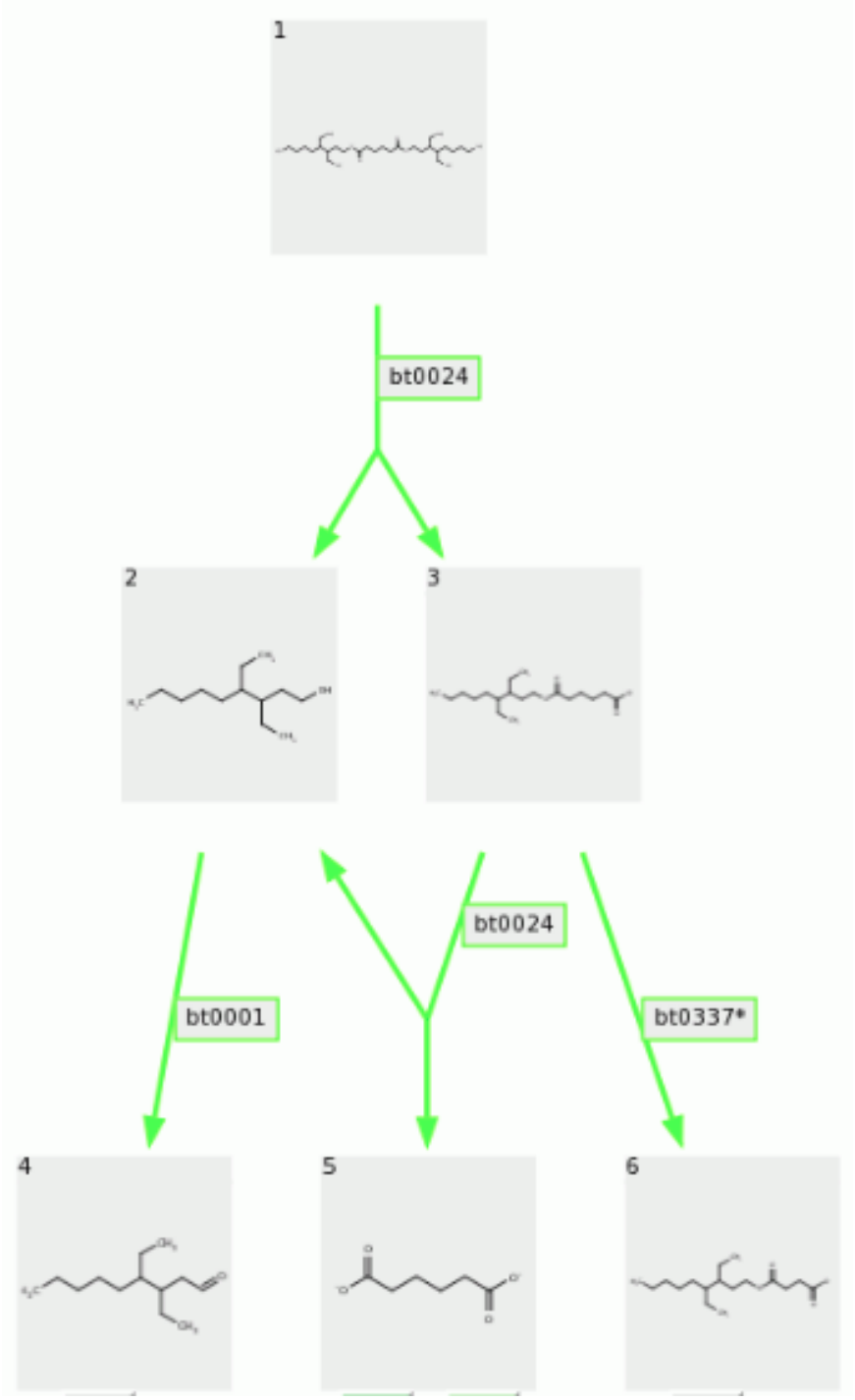


Figure 1. EAWAG Biodegradation pathway prediction (only the first levels included) of the representative isomer 1 (see table 5). The model predicts a similar pathway for all representative isomers of DITA.

Table 15 Screening tests

OVERVIEW OF AVAILABLE BIODEGRADATION STUDIES Method	Results	Remarks	Reference
Test type: ready biodegradability Activated sludge, domestic, non adapted. OECD Guideline 301 F (Ready Biodegradability: Manometric Respirometry Test)	Readily biodegradable (not meeting 10d window) 69% degradation of test substance within 28 days (CO_2 evolution)	1 (reliable without restrictions) key study experimental result Test material: diisotridecyl adipate	unnamed, (2014)
Test type: ready biodegradability Activated sludge, domestic, non adapted. OECD Guideline 301 F (Ready Biodegradability: Manometric Respirometry Test)	Not readily biodegradable % Degradation of test substance: 58.53 after 28 days (O_2 consumption) 11.57 after 6 days (O_2 consumption) 43.3 after 16 days (O_2 consumption)	1 (reliable without restrictions) supporting study experimental result Test material: diisotridecyl adipate	unnamed (2003)
Test type: ready biodegradability Activated sludge, domestic, non adapted OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test)	Readily biodegradable % Degradation of test substance: ca.81% after 28 days (CO_2 evolution) (after acidification)	2 (reliable with restrictions) supporting study experimental result Test material (EC name): diisotridecyl adipate	unnamed (2005)
Test type: ready biodegradability Activated sludge, domestic, non Adapted OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test)	Readily biodegradable failing the 10 day window % Degradation of test substance: 69.6 after 28 days (CO_2 evolution) 45.2 after 14 days (CO_2 evolution) 15.7 after 6 days (CO_2 evolution) 3.2 after 3 days (CO_2 evolution)	2 (reliable with restrictions) supporting study experimental result Test material (EC name): diisotridecyl adipate	unnamed (1999a)
Test type: ready biodegradability sewage, domestic, non adapted Equivalent or similar to USEPA Shake Flask method (EPA 560/6 82 003, CG 2000) Equivalent or similar to OECD Guideline 301 B (Ready Biodegradability: CO2 EvolutionTest)	Not readily biodegradable % Degradation of test substance: 56.6 after 29 days (CO_2 evolution) 40.6 after 14 days (CO_2 evolution) 18.2 after 5 days (CO_2 evolution) 3.6 after 2 days (CO_2 evolution)	2 (reliable with restrictions) supporting study experimental result Test material (EC name): diisotridecyl adipate	unnamed (1993)
Test type: inherent biodegradability Pre-exposed inocula equivalent or similar to ISO 14593	Inherently biodegradable % Degradation of test substance: ca. 65 after 56 days (CO_2 evolution)	2 (reliable with restrictions) supporting study experimental result Test material: diisotridecyl adipate	Battersby et al., (1999)

Several screening tests for ready or inherent biodegradability are available for diisotridecyl adipate (see Table 15). The OECD 301F study voluntarily performed by the registrants in 2014 (unnamed, 2014 – referred at the ECHA dissemination website) is considered to be the key study by the eMSCA. The source of the activated sludge was the municipal wastewater treatment plant "Breisgauer Bucht", Freiburg, Germany and it was confirmed that there was no possibility of pre-exposure of the activated sludge inoculum to oil or chemical products containing the substance. In the study, the degradation of diisotridecyl adipate reached 69% after 28 days. The criteria for 10-day window was not met but as the substance is a UVCB it is not considered necessary. No preadaptation of the inoculum was confirmed. Therefore, based on the results of this test, diisotridecyl adipate as a whole can be considered to be readily biodegradable.

In another OECD 301F test (unnamed, 2003 – referred at the ECHA dissemination website), 58.53 % degradation of the substance was observed after 28 days which is very close to the pass level (60 %).

Tests following or similar to OECD TG 301B (unnamed, 1993; 1999a; 2005 – referred at the ECHA dissemination website) are also available for the substance and 56.6-81 % degradation after 28-29 days is reported in these studies. However, according to the OECD 301 guideline, 301B is not applicable to volatile substances whereas 301F is applicable provided that precautions are taken to prevent volatilisation. No experimental information has been provided regarding volatility of DITA but, based on its physico-chemical characteristics the substance will volatilise from water. DITA volatilisation half-lives from both a model river and a lake are estimated to be ca. 0.2 and 10 days (Episuite v4.11), and Henry´s Law Constants (HLC) of 68.3-142 Pa·m^3/mol at 25ºC have been estimated for representative isomers of DITA by HENRYWIN v3.20 QSAR model (Episuite v4.1). These estimations agree with the water solubility of <0.001 mg/l and a HLC of 0.0007 atm·m^3/mol indicated for diisotridecyl adipate in a report by Comber and Holt (2010).

No threshold values for volatility are provided in the REACH Guidance documents or in the OECD test guidelines. But it is indicated that if HLC is greater than 100 Pa·m3/mol, more than 50% of the substance could be lost from the water phase in 3-4 hours (Guidance on Information Requirements and Chemical Safety Assessment, Chapter R.7b: Endpoint specific guidance, Version 4.0, June 2017; Table 7.8-2: Critical parameters for aquatic toxicity testing). Therefore, the OECD 301B test is not considered fully appropriate for DITA due to the potential volatility of the substance. However, as the degradation is measured based on CO_2 evolution, volatilisation of the test substance is expected to lead to a potential underestimation of the degradation instead of overestimation. Therefore, as pass level and near pass level were observed in the OECD 301B tests, they can be used as supporting information in the PBT assessment of DITA.

Information on the degradation of DITA is also available from a CONCAWE 1996/97 ring test of a CONCAWE method based on the ISO 14593 guideline with some modifications (Battersby et al., 1999) which involved 10 laboratories. The ISO 14593: Carbon dioxide (CO2) Headspace Biodegradation Test is a screening test for assessing the inherent aerobic biodegradability of organic substances. It is suitable for testing insoluble and/or volatile materials. The test is similar to that described in OECD 310, Ready Biodegradability – CO2 in sealed vessels (Headspace Test). In the CONCAWE ring test, inocula pre-exposed to the test substances were used and thus the test meets the definition of a test for inherent biodegradability. In the ring test, over half of the laboratories found DITA to be biodegraded by >60% based on theoretical inorganic carbon production (ThIC) after 56 days, and the overall mean biodegradation after 56 days was 65% ThIC. A relevant observation was that four of the six laboratories that reported >60% ThIC for DITA had collected their inocula from sites that had a known or suspected exposure to oil and chemical products. According to Pitter and Chudoba (1990), extensive biodegradation of branched compounds can occur if the population of microorganisms with adequate capabilities increases sufficiently during the pre-exposure period.

It is noted that some uncertainty regarding the ready biodegradability of the substance arise from the fact that DITA is recommended as a reference substance in the inherent guidelines OECD 302D (OECD, 2001), OPPTS 835.3215 (USEPA, 2008) and CEC L-33-A-93. The OPPTS and the OECD 302D guidelines state that to demonstrate the increased biodegradative power of the tests over a ready biodegradability test, di-isotridecyl adipate (DITA) can be used as a more difficult to biodegrade reference substance. These guidelines also quote the results from the above mentioned CONCAWE ring-test (Battersby et al 1999). Furthermore, based on information referenced in the Battersby et al (1999), DITA is typically biodegraded by only around 30% after 28 days with an unexposed inoculum (e.g. in OECD 301 B) but can be mineralised by 40 - 80% in the OECD 302D test.

Simulation tests

No relevant information available.

7.7.1.3.2. Biodegradation in soil

No relevant information available.

7.7.1.4. **Summary and discussion of degradation**

Based on the results of the most recent OECD 301F key study (69% degradation after 28 days based on CO_2 evolution) evaluated to be reliable by the eMSCA, diisotridecyl adipate as a whole substance is considered readily biodegradable. The high degradation level reached in this test indicate that the degradation is almost complete and that very little, if any, of the substance is left after 28 days. The near pass level (58.53 % degradation after 28 days) reached in an earlier test following the same guideline supports the conclusion of rapid biodegradability. Furthermore, 56.6-81 % degradation observed in OECD 301B tests also indicate that the substance is readily/rapidly biodegradable although this guideline is not considered fully appropriate for the substance due to volatility of DITA.

As the substance is a UVCB consisting of several constituents and some of them can be present at low concentrations, a firm conclusion on the degradation of all possible constituents cannot be made based on the tests performed with the whole substance. Therefore, BIOWIN QSAR models were performed for isomers representing the most common structures as well as theoretical worst case structures. Based on the BIOWIN predictions, isomers with higher degree of branching (at least 5 branches in total in the two sidechains) and/or with quaternary carbons may be potentially persistent. However, it is noted that taking into account the available information on the composition of the substance, the presence of constituents with quaternary carbons is unlikely.

Furthermore, based on the BIOWIN 4 model and the biodegradation pathway predictions, primary degradation through cleavage of the ester bonds may occur leading to the formation of adipic acid and isotridecyl alcohols. Based on the available information, these degradation products are readily biodegradable.

In conclusion, most of the isomers of the substance are considered to be readily biodegradable based on the high level of degradation observed in the ready biodegradation tests with the whole substance and the BIOWIN QSAR predictions performed for representative isomers. Some uncertainty remains regarding the degradation of isomers with higher degree of branching, and based on the available information it is not possible to firmly conclude on their persistence. However, relatively rapid primary degradation might be expected for all isomers, and the expected degradation products are not persistent. Hence, all isomers of DITA are likely to be non-persistent.

7.7.2. Environmental distribution

7.7.2.1. **Adsorption/desorption**

The Koc of diisotridecyl adipate was estimated with the EPI Suite KOCWIN (v2.00) QSAR model using the smiles of the representative isomers as input (see Table 16). Using a correlation based on molecular connectivity index (MCI), the log Koc was determined to be in the range of 6.86-7.16 depending on the smiles used. Using a correlation based on Kow, the log Koc values of the isomers were in the range of 7.84-8.00. Hence, the isomers of the substance are expected to adsorb to soil.

Table 16

KOCWIN QSAR PREDICTIONS FOR REPRESENTATIVE ISOMERS OF DITA		
Isomer*	Log Koc (MCI method)	Log Koc (log Kow method)
1	7.11	7.92
2	7.16	8.00
3	6.90	7.84
4	7.01	7.92
5	7.12	8.00
6	7.01	7.88
7	6.86	7.86
8	6.84	7.92

* See Table 5 for further information on the representative isomers.

The McCall classification scheme classifies the substance as immobile in soil (Koc>5000).

The following information is taken into account for any environmental exposure assessment:

An average value of Log Koc 7.05 (MCI method) is calculated based on the predicted log Koc values of the representative isomers representing the most common structures (isomers 1-6 in table 16).

7.7.2.2. **Volatilisation**

No experimental information has been provided regarding volatility of DITA but, according to its physico-chemical characteristics the substance will volatilise from water. Henry´s Law Constants (HLC) at 25ºC have been estimated by HENRYWIN v3.20 QSAR model (Episuite v4.1) using the smiles of the representative isomers as input (see Table 17).

Table 17

HENRYWIN QSAR PREDICTIONS FOR REPRESENTATIVE ISOMERS OF DITA		
Isomer*	HLC (Bond contribution method)	HLC (Group contribution method)
1	88.9	98.7
2	88.9	68.3
3	88.9	143
4	88.9	98.7
5	88.9	68.3
6	88.9	119
7	88.9	119
8	88.9	82.1

* See Table 5 for further information on the representative isomers.

These estimations agree with the water solubility of <0.001 mg/l and a HLC of 0.0007 atm·m^3/mol (70.95 Pa·m^3/mol) indicated for diisotridecyl adipate in a report by Comber and Holt (2010).

An average value of 92.33 Pa·m^3/mol (at 25°C) is calculated based on the predicted values (bond and group contribution methods) of the isomers representing the most common structures (isomers 1-6 in table 18) and the value reported by Comber and Holt (2010). In the risk assessment a Henry's Law Constant at 12 °C is used. This was calculated by EUSES using the average value of 92.33 at 25 °C as input, which resulted in a HLC of 44.2 at 12 °C.

In conclusion, based on the available information, the substance is moderately volatile from water (10^{-3} – 10^{-5} at·m3/mol)[4].

[4] The ranges of HLC values and the information they provide about the chemical are shown below. HLC value (atm-m^3/mole) Classification: > 10^{-1} Very volatile from water; 10^{-1} - 10^{-3} Volatile from water; 10^{-3} - 10^{-5} Moderately volatile from water; 10^{-5} - 10^{-7} Slightly volatile from water < 10^{-7} Non volatile.

7.7.2.3. **Distribution modelling**

Environmental distribution has been predicted with the Episuite v4.1 distribution modelling using the smiles of the representative isomers as input (see Table 5) and assuming equal emissions to air, water and soil (see Table 18).

Table 18

EPISuite LEVEL III FUGACITY MODEL PREDICTIONS FOR REPRESENTATIVE ISOMERS OF DITA				
Isomer*	Air (%)	Water (%)	Soil (%)	Sediment (%)
1	0.43	22.2	77.3	0.02
2	0.44	22.1	77.5	0.02
3	0.20	16	83.7	0.03
4	0.44	22.1	77.4	0.02
5	0.44	22	77.5	0.02
6	0.19	16	83.8	0.03
7	0.14	12.4	87.5	0.02
8	0.15	12.1	87.7	0.02

* See Table 5 for further information on the representative isomers.

7.7.3. Bioaccumulation

7.7.3.1. **Aquatic bioaccumulation**

The studies on aquatic bioaccumulation are summarised in the following table:

Table 19

OVERVIEW OF AVAILABLE AQUATIC BIOACCUMULATION DATA			
Method	**Results**	**Remarks**	**Reference**
Lepomis macrochirus aqueous (freshwater) flow through. Total uptake duration: 28 d Total depuration duration: 14 d U.S. EPA and ASTM procedures	BCF: 27	3 (not reliable) (structural analogue or surrogate) Test material (CAS name): **Bis(2-ethylhexyl) adipate**	BUA (1996) SIDS (2000) Felder, et al (1986)
Details on estimation of bioconcentration: BASIS FOR CALCULATION OF BCF Estimation software: OASIS Catalogic v5.11.6TB [BCF base line model v.02.05 (new ionization term] INPUT DATA USED BY THE MODEL: log Kow: 16.76 (KOWWIN v1.68 estimate) Water solubility: 2.457E 012 mg/L (WSKOW v1.42 estimate) Calculation using Catalogic v.5.11.6TB, BCF base line model v.02.05 (new ionization term)	BCF: 24.55 (Without considering the mitigating factors size, metabolism and water solubility) log BCF: 1.39 (± 0.17; without considering the mitigating factors size, metabolism and water solubility) BCF: 7.08 (Considering the mitigating factors size, metabolism and water solubility) log BCF: 0.85 (± 0.11; Considering the mitigating factors size, metabolism and water solubility)	3 (not reliable) estimated by calculation (EC name: diisotridecyl Adipate)	unnamed (2013 referred at the ECHA website) Dimitrov et al., (2005)

No experimental bioaccumulation test is available for DITA. The constituents of the substance have high estimated log Kow values in the range of 12.73-13.03 which are above the cut-off value of 10 for limited bioaccumulation potential indicated in REACH Guidance on Information Requirements and Chemical Safety Assessment, Chapter R.11: PBT/vPvB assessment, Version 3.0, June 2017. The BCFBAF v3.01 (EPI Suite v4.00) QSAR programme predicts BCF values in the range of 14.8-20.7 based on the log Kow method and BCF values around 1 based on the Arnot-Gobas method (see Table 20). This suggests that the constituents of the substance may have limited potential for bioaccumulation.

Simulations based on OASIS model has been considered not reliable since there is no information on the isomers nor the SMILES used to run the model.

Table 20

BCFBAF QSAR PREDICTIONS FOR REPRESENTATIVE ISOMERS OF DITA			
Isomer*	BCF (Log Kow method)	BCF (A-G method with biotransformation)	BCF (A-G method with zero biotransformation)
1	17.5	0.8948	1.005
2	14.8	0.8944	0.9731
3	20.7	0.895	1.051
4	17.5	0.8948	1.005
5	14.8	0.8944	0.9731
6	19	0.8949	1.026
7	19.8	0.8954	1.038
8	17.5	0.8958	1.006
9	19.1	0.8962	1.027
10	19.1	0.8959	1.027
11	18.3	0.8965	1.016

* See Table 5 for further information on the representative isomers.

Molecular size and weight can also be used in a weight of evidence assessment to strengthen the evidence of limited bioaccumulation potential. Very bulky molecules may have hindered uptake leading to lower BCF values. According to the registration information, the calculated mean maximum diameter of the constituents of DITA is 25.75 Å and the lowest maximum diameter calculated for the 30 energetically preferred 3D structures of the substance is 18.16 Å. These are over 17.4 Å considered as cut-off for not likely to meet the criteria for B according to REACH Guidance on Information Requirements and Chemical Safety Assessment, Chapter R.11: PBT/vPvB assessment, Version 3.0, June 2017. Also the molecular weight of DITA (510 g/Mol) is relatively close to the cut-off value (700 g/Mol) considered for hindered up-take. There is no information on the molecular length of the constituents of DITA but it does not seem likely that the linear or branched structure of the molecule could be easily transferable across cell membranes. Therefore, based on the molecular size and structure of the isomers of DITA their potential to cross biological membranes can be expected to be limited.

In the registration dossier of DITA a bioconcentration test on the similar substance bis(2-ethylhexyl) adipate (DEHA) performed following U.S. EPA and ASTM procedures and using bluegill sunfish (*Lepomis macrochirus*) as test organisms (Felder et al., 1986) is included. The eMSCA considers that direct read across from DEHA to DITA is not possible in bioaccumulation assessment as DEHA is a monoconstituent substance with C8 chains as sidechains whereas DITA is a UVCB substance with C13 sidechains and DEHA has a lower log Kow (measured value 8.94, predicted value 8.12) and a higher water solubility (0.0032 mg/L) than the isomers of DITA. Furthermore, the test concentration used in the bioaccumulation study (250 µg/L) was two orders of magnitude higher than the water solubility of DEHA, and therefore, the BCF value of the study is not considered reliable. Consequently, the study was not taken into account by the eMSCA in the bioaccumulation assessment of DITA.

Toxicokinetics studies on mammals are available for DEHA (see section 7.9.1). As explained above, direct read across is not possible between these substances in bioaccumulation assessment but the toxicokinetic information on DEHA is used as supporting information. Based on that information, DEHA and/or its metabolites are readily absorbed from the gastrointestinal tract but their excretion is also rapid and extensive. Furthermore, DEHA appears to be rapidly metabolised and only low levels of DEHA were detected in tissues and organs. There was no evidence of accumulation of radioactivity in any organ or tissues. Especially the information indicating that the ester bonds in DEHA are quickly metabolised in mammals is relevant for the bioaccumulation assessment of DITA as a similar metabolisation pathway may be expected for these substances.

7.7.3.2. **Terrestrial bioaccumulation**

There is no relevant experimental information available.

EPISuite KOAWIN (v1.10) QSAR model predicts log Koa values of ca. 14 for the representative isomers of DITA included in Table 5. Therefore, the predicted log Kow and log Koa values of the isomers fulfill the screening criteria for potential to biomagnify in air-breathing organisms indicated in the REACH Guidance on Information Requirements and Chemical Safety Assessment, Chapter R.11: PBT/vPvB assessment (Version 3.0, June 2017).

7.7.3.3. **Summary and discussion of bioaccumulation**

No experimental bioaccumulation test is available for DITA. The predicted log Kow values of the constituents are above the cut-off value of 10 suggesting limited potential for bioaccumulation and the predicted BCF values are very low. In addition, based on the high molecular size of the constituents hindered uptake and low BCF values may be expected.

Furthermore, toxicokinetic data available for the similar substance DEHA suggests that the constituents of DITA may be rapidly metabolised through cleavage of the ester bond, at least in mammals. (See section 7.9.1 below).

In conclusion, using the weight-of-evidence approach and considering the potential hindered uptake based the very high log Kow values (above 10) and molecular size as well as the low predicted BCF values and the potential rapid metabolism, the constituents of DITA are not expected to have a high bioaccumulation potential.

7.8. Environmental hazard assessment

7.8.1. Aquatic compartment (including sediment)

7.8.1.1. Fish

There is only acute toxicity data available for fish. The available studies are summarised in the following table:

Table 21.

OVERVIEW OF AVAILABLE SHORT-TERM TOXICITY STUDIES ON FISH			
Method	**Results**	**Remarks**	**Reference**
Poecilia reticulata freshwater static OECD Guideline 203 (Fish, Acute Toxicity Test) (adopted 17 July 1992)	LL50 (96 h): > 100 mg/L test mat. (nominal) based on: mortality	3 (not reliable) supporting study experimental result Test material (EC name): diisotridecyl adipate	unnamed (1998a) (referred at the ECHA´s website)
Cyprinodon variegatus saltwater static equivalent or similar to OECD Guideline 203 (Fish, Acute Toxicity Test)	LC50 (96 h): > 5000 mg/L test mat. (nominal) based on: mortality (only 4 of 20 test animals died at the highest test concentration (5000 ppm))	3 (not reliable) supporting study experimental result Test material (EC name): diisotridecyl adipate	unnamed (1986) (referred at the ECHA´s website)

The acute lethal toxicity of diisotridecyl adipate to *Poecilia reticulata* (Guppy) was investigated under static exposure conditions over a period of 96 h. The only applied nominal test concentration was 100 mg/l. This is far above the water solubility of the substance, and an oily layer was observed on the surface of the test medium. None of a total of seven fish died after 96 h of exposure. Other toxic effects than mortality, e.g. loss of coordination, hypo or hyperactivity and swimming on the back, were not observed. A NOEC of ≥ 100 mg/l and a 96h LL50 of > 100 mg/l (nominal concentration) are reported (unnamed, 1998a – referred at the ECHA´s website).

Additionally, a study with sheepshead minnows (*Cyprinodon variegatus*) in salt water is available. In a 96 h acute toxicity study, groups of 20 sheepshead minnows were exposed to diisotridecyl adipate at nominal concentrations of 0 (control), 500, 1000, 2500, and 5000 mg/L in 38 L glass vessels under static conditions. Fish were exposed to an emulsion of test substance in test medium (30 L artificial sea water, salinity 20 ppt). Diesel oil (300 mg/L) was used as positive control. Mortality was only observed in the highest dose group (4 of 20 animals). As the test concentrations were far above the water solubility limit of the substance, the observed mortality may be caused by physical effects of undissolved test material. Sublethal effects could not be noticed due to the opacity of the test medium (emulsion of test substance in test water). The 96 h LC50 was determined to be > 5000 mg/L (unnamed, 1986 – referred at the ECHA´s website).

The nominal test concentrations were well above the water solubility of diisotridecyl adipate (< 0.001 mg/L), and therefore, the studies are not considered reliable. However, they suggest that there may not be any acute effects to fish at the water solubility limit of the substance.

No relevant studies on long-term toxicity to fish are available.

The following information is taken into account for acute fish toxicity for the derivation of PNEC:

No reliable studies are available but there seems to be no acute effects to fish at the limit of water solubility of diisotridecyl adipate.

7.8.1.2. **Aquatic invertebrates**

Short-term toxicity:

The available acute toxicity studies on aquatic invertebrates are summarised in the following table:

Table 22.

OVERVIEW OF AVAILABLE SHORT-TERM TOXICITY STUDIES ON AQUATIC INVERTEBRATES			
Method	**Results**	**Remarks**	**Reference**
Daphnia magna freshwater static OECD Guideline 202 (Daphnia sp. Acute Immobilisation Test) (Part 1, adopted 25 April 1984)	EL50 (48 h): > 1000 mg/L test mat. (nominal) based on: mobility (tested as water accommodated fraction)	3 (not reliable) supporting study experimental result Test material (EC name): diisotridecyl adipate	unnamed (1998b)
Daphnia magna freshwater static equivalent or similar to OECD Guideline 202 (Daphnia sp. Acute Immobilisation Test)	EC50 (48 h): > 500 mg/L test mat. (nominal) based on: mobility	3 (not reliable) supporting study read across from supporting substance Test material (EC name): bis(2-ethylhexyl) adipate	unnamed (1988)
Daphnia magna freshwater static EU Method C.2 (Acute Toxicity for Daphnia) OECD Guideline 202 (Daphnia sp. Acute Immobilisation Test (adopted: 4. April 1984)	EC50 (24 h): 4800 mg/L test mat. (nominal) based on: mobility	3 (not reliable) supporting study experimental result Test material (EC name): diisotridecyl adipate	unnamed (1997)

To assess the short term toxicity of diisotridecyl adipate to aquatic invertebrates, three tests with *Daphnia magna* are available; two with DITA and one with the similar substance DEHA.

The acute toxicity of diisotridecyl adipate to *Daphnia magna* was investigated according to OECD Guideline 202 (Part 1, adopted 25 April 1984) under static exposure condition

over a period of 48 h using water accommodated fractions (WAF). Two loading rates of 100 and 1000 mg/l were tested. The WAFs were prepared by moderately stirring the test substance in test medium for 24 h at room temperature, and after this the undissolved materials were removed by filtration (MILLIPORE glass fibre filter AP15). The concentrations of the test substance in the WAFs were not measured. At the loading rate of 1000 mg/l 17.5 % of Daphnia were immobile after 48 h of exposure. At 100 mg/l 10 % immobile Daphnia were observed after 48 h of exposure. Based on the results of the study it can be concluded that the 48 h EL50 value of diisotridecyl adipate is >1000 mg/l nominal concentration (unnamed, 1998 – referred at the ECHA´s website). However, the study is not considered reliable as the loading rates were well above the water solubility limit and the actual exposure concentrations in the WAFs were not measured.

The second acute test with DITA (1997) is not considered appropriate and reliable for the assessment as the test duration was only 24 hours and there is limited information available on the test, e.g. on the number of animals used.

The 48 h acute toxicity of bis(2-ethylhexyl) adipate to water fleas was studied under static conditions in a Daphnia magna immobilisation test similar to OECD test guideline 202 (unnamed, 1988 – referred at the ECHA´s website). Daphnids were exposed to nominal concentrations of 0 (control), 15.62, 31.2, 62.5, 125, 250, and 500 mg/L test substance. To increase solubility a vehicle was used (Tween 80,100 mg/L). In controls and vehicle controls, no immobilisation of daphnids was observed. The 48 h EC50 based on immobilisation was determined to be > 500 mg/L (unnamed, 1988). The nominal concentrations used in the test are far above the water solubility of DEHA (0.0032 mg/L), and there is no information on the actual exposure concentrations. Therefore, the test is not considered reliable.

The following information is taken into account for short term toxicity to aquatic invertebrates for the derivation of PNEC:

No reliable studies are available. In the study using WAFs effects were observed and a 48 h EL50 value of >1000 mg/l loading rate is reported. However, the loading rates were well above the water solubility of the substance and there is no information on the actual exposure concentrations. Therefore, this result cannot be used in the PNEC derivation.

Long-term toxicity:

The available chronic toxicity studies with DITA and the read across substances are summarised in the following table:
Table 23.

OVERVIEW OF AVAILABLE LONG-TERM TOXICITY STUDIES ON AQUATIC INVERTEBRATES			
Method	**Results**	**Remarks**	**Reference**
Daphnia magna freshwater semi static OECD Guideline 211 (Daphnia magna Reproduction Test)	NOEC (21 d) = 0.0016 mg/L test mat. (meas. (TWA)) based on: reproduction)	2 (reliable with restrictions) key study Test material: (EC name) diisotridecyl adipate	unnamed (2016)
Daphnia magna freshwater semi static OECD Guideline 211 (Daphnia magna Reproduction Test) (Cited as OECD Guide line 202, part 2 (Daphnia sp., Reproduction Test))	NOEC (21 d): >= 0.77 mg/L test mat. (meas. (geom. mean)) based on: reproduction LOEC (21 d): > 0.77 mg/L test mat. (meas. (geom. mean))	3 (not reliable). Solvent used has been referred as promoting young in daphnia reproduction tests read across from supporting substance (structural analogue or surrogate) Test material (EC name): bis(2- ethylhexyl) adipate	unnamed (1996a)
Daphnia magna freshwater flow through ASTM E47.01 (American Society for Testing and Materials)	21 d: NOEC: 0.024 LOEC: 0.052 mg/L. based on: mean length, survival and reproduction	2 (reliable with restrictions) key study read across from supporting substance (structural analogue or surrogate) Test material (EC name): bis(2-ethylhexyl) adipate	BUA (1996) SIDS (2000) Felder et al., (1986)
Daphnia magna freshwater semi static OECD Guideline 211 (Daphnia magna Reproduction Test) ASTM Method E 1193 097	NOEC (21 d): 5 µg/L test mat. (meas. (initial)) based on: reproduction NOEC (21 d): 5 µg/L test mat. (meas. (initial)) based on: growth NOEC (21 d): 5 µg/L test mat. (meas. (initial)) based on: mortality	2 (reliable with restrictions) supporting study read across from supporting substance (structural analogue or surrogate) experimental result Test material (EC name): bis(2-ethylhexyl) adipate	Robillard et al, 2008)
Daphnia magna OECD 211 (Daphnia magna Reproduction Test) GLPs	No toxic effect at the limit of water solubility. NOEC and LOEC: 0.00063 mg/L	3 (not reliable) Insufficient data to adequately quantify the exposure. read across from supporting substance (structural analogue or surrogate) Test material: diisotridecyl dodecanedioate (CAS Nº: 84731-63-5)	unnamed (2013).

In 2016 the registrants provided a new 21-d Daphnia magna reproduction study with DITA following the OECD test guideline 211, as requested in the SEV decision. Due to the

low water solubility of DITA, the test solutions were prepared using a column elution method. Young female daphnids (less than 24 hours old) were exposed under semi-static conditions to two test concentrations: a steady state column eluate in form of the 100% eluate and 1:10 dilution of the eluate (10 % eluate). The concentrations of the test substance in the eluate and in the dilution of the eluate were measured upon test solution renewal on each working day. The time weighted average concentrations of the test substance were 17.22 μg/L (100% eluate) and 1.60 μg/L (10 % eluate). Undissolved test substance was not detected in the visual examination of the test solutions but micelle formation could be possible as the higher concentration is above the water solubility (0.7 μg/L) measured for the substance in deionised water in an OECD 105 test using the column elution method. However, as the substance is a UVCB and the dissolution water used in the daphnia test (purified drinking water) was different than in the OECD 105 test (deionised water), the eMSCA concluded that the test concentrations can be considered to fall in the range of water solubility of the substance.

The treatment groups were compared to the control group in regard to the total number of living offspring produced per surviving parent animal, age at first reproduction, mobility, length and intrinsic rate of increase. In the 10% eluate treatment group no significant effects in daphnia were observed. In the 100% eluate group, a 27% reduction in the mean number of cumulative offspring per surviving daphnids after 21 days were seen. Hence, a NOEC of 1.60 μg/L is reported.

In the registration dossier, four studies with read across substances are also included. Two of them are considered as supporting information in the assessment but the other two are not taken into account in the assessment as one of them is not considered reliable and the reliability of the other one cannot be assigned.

The 21 day *Daphnia magna* reproduction test according to OECD test guideline 211 (1984, part 2) with bis(2-ethylhexyl) adipate (DEHA) is not considered reliable for this assessment. On the one hand, the daphnids were exposed to nominal concentrations of 0.5, 1.0, and 2.0 mg/L of the test substance (measured concentrations 0.19, 0.39, and 0.77 mg/L). During the test, no effects were observed, and a NOEC of >= 0.77 mg/L was determined for DEHA. Thus, the lowest concentration tested (0.5 mg/L) and the reported NOEC (0.77 mg/L) are x100 times above the limit of solubility of DEHA. On the other hand, to solubilise the test substance, MARLOWET R 40 was used as a vehicle (1g/L). Separate studies with this dispersants confirm the observation that "Marlowet R40" promotes the number of young produced in Daphnia reproduction tests[5]. Therefore, its use as a solvent in reproduction tests may have an impact on the test result. Based on these considerations, this test was not considered reliable for the assessment.

Robillard et al. (2008) performed a chronic Daphnia magna limit test with DEHA at an average exposure of 4.4 µg/L in laboratory diluent water to avoid insoluble test material and avoid physical entrapment. In the same study, the authors report a measured water solubility of 5.5 µg/L using the slow-stir method. One hundred percent of the DEHA treated organisms survived compared to 90% survival in both the controls and solvent controls. Mean neonate reproduction was 152, 137, and 148 and mean dry weight per surviving female was 0.804, 0.779, and 0.742 mg in the treatment, control and solvent control, respectively. No adverse effects were observed. Information from this limit test is considered as additional supporting information for DITA.

The third study (Felder et al., 1986) is a 21-d flow-through *Daphnia magna* chronic test on DEHA conducted following American Society for Testing and Materials (ASTM)

[5] ECHA, 2011. Annex XV. Restriction report proposal for a restriction substance name: Bis(2-ethylhexyl)phthlate (DEHP), Benzyl butyl phthalate (BBP), Dibutyl phthalate (DBP), Diisobutyl phthalate (DIBP). http://echa.europa.eu/documents/10162/c6781e1e-1128-45c2-bf48-8890876fa719

procedures[6]. Test methodology and procedure were well described including treatment and controls in quadruplicate. Five concentrations of DEHA were tested (from 0.014 mg/L to 0.180 mg/L) at a maximum concentration of 0.2 mg/L of acetone as solvent. The lowest measured concentration was 0.014 mg/L, which is within a factor of 5 of the two water solubility values measured for DEHA (0.0055 and 0.0032 mg/L). The maximum concentration of acetone in the final test medium (0.2 mg/L) did not exceed the corresponding toxicity thresholds recommended for this solvent: Acetone at 100 µl/L (equivalent to 0.79 mg/L) (OECD, 2000[7]). Additionally, Hutchinson et al (2006) published a review of effects of solvents, including acetone, in which it is concluded that reproductive effects are unlikely to occur in daphnids at concentrations within current solvent concentration guidelines.

The authors of the Felder et al (1986) study concluded a measured NOEC of 0.024 mg/L and a measured LOEC of 0.052 mg/L. Chronic effects to daphnids were reported including immobilisation, reduced lengths, and reduced young per adult per day at measured test concentrations above 0.052 mg/L. Hence, no effects were observed below the water solubility of the test substance. Where effects were observed above the water solubility it is unclear whether physical effects occurred. This means the results of the study are uncertain. It is also noted that there may be uncertainties in the measurements of the low concentrations used in the study. Nevertheless, based on this study, potential adverse effects of DEHA on daphnia at concentrations slightly above its water solubility limit (x7) can be expected. This supports the results of the OECD 211 study performed with DITA where chronic toxicity was observed.

On November, 2013, registrants sent a new study (unnamed, 2013 – referred at the ECHA´s website) with a second read-across substance, the UVCB substance diisotridecil dodecanedioate. The test was performed according to the OECD 211 Guideline. Nevertheless, the study is considered not assignable by the eMSCA due to uncertainties in the preparation of the solution exposure concentrations. According to the information provided in the study, the analysis of the freshly prepared 100% v/v solution preparation from days 0 to 19 showed measured concentration ranging from less than the Limit of Quantification (L0Q =0.00027 mg/L) to 0.0024 mg/L at day 5 of the 21d exposure period, which is considered by the registrant(s) as a saturation concentration. However, uncertainties on this point arise. According to the information this concentration is the maximum concentration measured, but there is no guarantee of being the maximum concentration attainable by the substance.

Additionally, this maximum measured concentration was not kept constant during the exposure period. In fact, an overall decline in the measured concentrations is recognised between each period of media renewal (three times per week). A high variation on the exposure concentrations is indicated during the 21 days exposure period, being most of the concentrations below the L0Q. Concentration of 0.0024 mg/L was only determined at day 5 corresponding to the days 5 to 7 of the exposure period. In fact, the EC values of the study are referred to the mean worst case measured concentrations (0.00063 mg/L).Therefore, there is no guarantee that the observed "no effects" were due to the lack of toxicity or due to the lack of test substance, since volatilisation and losses of components by filtration processes cannot be excluded. This study provides insufficient reliability to adequately quantify the exposure concentrations tested.

In conclusion, chronic effects in the reproduction of daphnia were observed in the OECD 211 study with DITA at a concentration that can be considered to be in the water

[6] American Society for Testing and Materials Task Group on Daphnids. 1981. Proposed standard practice for conducting Daphnia magna chronic toxicity tests in a flow-through system. Draft No. 3. ASTM E-47.01 American Society for Testing and Materials, Philadelphia, PA.

[7] The OECD recommends a maximum solvent concentration of 100 µl/l (with specific gravity equivalents to 100 µl l^{-1} in parentheses) for acetone (79 mg/l), dimethylformamide (95 mg/l), dimethylsulfoxide (1.10 mg/l), ethanol (78.9 mg/l), methanol (79.2 mg/l) and triethylene glycol (1.12 mg/l). OECD Series on testing and assessment. Number 23. Guidance Document on Aquatic Toxicity Testing of Difficult Substances and Mixtures. http://www.epa.gov/endo/pubs/ref-2_oecd_gd23_difficult_substances.pdf

solubility range of the substance. The study resulted in a NOEC of 0.0016 mg/L. It is noted that only two concentrations were tested in the study and the separating factor between the concentrations was 10. However, this NOEC is considered for the risk assessment as a worst-case NOEC. Potential long-term effects in daphnia observed for the read-across substance DEHA (mono-constituent substance) at concentrations slightly above its measured water solubility support the conclusion that long-term effects can be expected to DITA. It is also noted that DITA is a mixture of complex isomers of the isotridecyl carbon chain. The alcohol has more than 50 possible isomers. The metabolites of DITA, alcohols, C11-14-iso-, C13-rich, such as isotridecyl alcohol are known to exert toxicity on aquatic organisms (ECHA´s dissemination website, 2017b). These alcohols act by non-polar narcosis and a similar order of magnitude of toxicity in fish, invertebrates and algae will be expected.

7.8.1.3. **Algae and aquatic plants**

The available toxicity studies on algae are summarised in the following table:

Table 24.

OVIERVIEW OF AVAILABLE TOXICITY STUDIES ON ALGAE AND AQUATIC PLANTS			
Method	**Results**	**Remarks**	**Reference**
Desmodesmus subspicatus (reported as Scenedesmus subspicatus) (algae) freshwater static OECD Guideline 201 (Alga, Growth Inhibition Test) (adopted 7 June 1984)	EL50 (72 h): > 1000 mg/L test mat. (as water accommodated fraction) (nominal) based on: growth Rate. NOELR (72 h): >= 100 mg/L test mat. (as water accommodated fraction) (nominal) based on: growth Rate.	3 (not reliable) supporting study experimental result Test material (EC name: diisotridecyl adipate)	unnamed (1998)
Scenedesmus subspicatus (new name: Desmodesmus subspicatus) (algae) freshwater static EU Method C.3 (Algal Inhibition test)(Version May 1988 (79/831/EWG, Annex V))	EC50 (72 h): 68 mg/L test mat. (nominal) based on: growth rate EC50 (72 h): 45 mg/L test mat. (nominal) based on: biomass EC10 (72 h): 24 mg/L test mat. (nominal) based on: growth rate EC10 (72 h): 14.9 test mat.(nominal) based on: biomass	3 (not reliable) supporting study experimental result Test material (EC name: diisotridecyl adipate)	unnamed (1990)

In a study following OECD 201 guideline, the toxicity of DITA to *Desmodesmus subspicatus* was assessed for a period of 72 h using water accommodated fractions (WAF) at loading rates of 100 and 1000 mg/l. The test substance in concentrations of 100 and 1000 mg/l were moderately stirred in algal medium for 24 h at room temperature, and after this the undissolved materials were removed by sterile filtration (0.45µm). The resulting WAFs were used in the test. The EL50 (24-72 h) of diisotridecyl adipate based on the growth rate was > 1000 mg/l nominal loading rate and the NOELR

based on the growth rate was >= 100 mg/l nominal loading rate (unnamed, 1998 – referred at the ECHA´s website). The loading rates were well above the water solubility limit of the substance and the concentration of the test substance in the test solutions was not analytically measured. Therefore, the study is not considered reliable.

In another study considered not reliable (unnamed, 1990 – referred at the ECHA´s dissemination website), EC50 and EC10 values far above the water solubility of diisotridecyl adipate and based on nominal concentrations are reported.

The following information is taken into account for effects on algae / cyanobacteria for the derivation of PNEC:

In an algal inhibition test with diisotridecyl adipate as test substance it was concluded that the EL50 (24-72 h) based on the growth rate is > 1000 mg/l nominal loading rate and the NOELR based on the growth rate is ≥ 100 mg/l nominal loading rate. As the nominal loading rates are far above the water solubility limit of the substance and the actual exposure concentrations were not analytically measured, this information cannot be used for PNEC derivation.

7.8.1.4. **Sediment organisms**

Information on effects on sediment organisms has been provided on the read across substance diisooctyl adipate.

A 10-day sediment test was performed on the similar substance diisooctyl adipate (EC: 215-553-5; CAS: 1330-86-5), with the amphipod *Leptocheirus plumulosus*, following EPA-821-R-11-004 (consistent with ASTM Standard Guide E 1367 Standard Test method for measuring the short-term toxicity of sediment-associated contaminants with marine and estuarine invertebrates). The 10d-LC50 was > 12000 mg/kg and the NOEC 4000 mg/kg.

7.8.1.5. **Other aquatic organisms**

No relevant information available.

7.8.2. Terrestrial compartment

7.8.2.1. **Toxicity to soil macro-organisms**

The available toxicity studies on soil macro-organisms are summarised in the following table:

Table 25

OVERVIEW OF AVAILABLE TOXICITY STUDIES ON SOIL MACRO-ORGANISMS			
Method	**Results**	**Remarks**	**Reference**
Eisenia fetida (annelids) short term toxicity laboratory study) Substrate: artificial soil EU Method C.8 (Toxicity for Earthworms: Artificial Soil Test) (Cited as Directive 87/302/EEC, part C, p. 95 (Toxicity for earthworms: Artificial soil test))	NOEC (14 d): 550 mg/kg soil dw test mat. (nominal) based on: mortality LC50 (7 d): > 1000 mg/kg soil dw test mat. (nominal)based on: mortality LC50 (14 d): 865 mg/kg soil dw test mat. (nominal)based on: mortality (550- 1000 mg/kg)	2 (reliable with restrictions) key study read across from supporting substance (structural analogue or surrogate) Test material (IUPAC name): bis(2-ethylhexyl) adipate	unnamed (1996)
Eisenia fetida [Annelida] (annelids) short-term toxicity Substrate: artificial soil according to OECD Guideline 207 (Earthworm, Acute Toxicity Tests) ; according to EU Method C.8 (Toxicity for Earthworms: Artificial Soil Test)	NOEC (14 d) > 1000 mg/kg soil dw (nominal) based on: mortality LC50 (14 d): >1000 mg/kg soil dw (nominal) based on: mortality	2 (reliable with restrictions) read across from supporting substance (structural analogue or surrogate) Test material (IUPAC name): bis(tridecyl) adipate (EC 241-029-0)	unnamed (2012)

No experimental information on toxicity to soil macro-organisms of diisotridecyl adipate is available. Only short-term information from two read across substances is available. The lowest LC50 of the read across substance bis(2 ethylhexyl) adipate after 14 d was 865 mg/kg soil (unnamed, 1996 – referred at the ECHA´s website).

The following information is taken into account for effects on soil macro organisms except arthropods for the derivation of PNEC:

The LC50 of the read across substance bis(2 ethylhexyl) adipate after 14 d was 865 mg/kg soil.

7.8.2.2. **Toxicity to terrestrial plants**

No relevant information is available.

7.8.2.3. **Toxicity to soil micro-organisms**

No relevant information is available.

7.8.3. Microbiological activity in sewage treatment systems

The available information on the effects on micro-organisms of sewage treatment systems is summarised in the following table:

Table 26

OVERVIEW OF AVAILABLE STUDIES ON TOXICITY TO STP MICROORGANISMS			
Method	**Results**	**Remarks**	**Reference**
activated sludge EU Method C.11 (Biodegradation: Activated Sludge Respiration Inhibition Test) (Cited as Directive 87/302/EEC, part C, p. 118 (Biodegradation: Activated sludge respiration inhibition test))	NOEC (3 h): > 350 mg/L test mat. (nominal) based on: respiration rate EC50 (3 h): > 350 mg/L test mat. (nominal) based on: respiration rate	2 (reliable with restrictions) key study read across from supporting substance (structural analogue or surrogate) Test material (EC name): bis(2-ethylhexyl) adipate	ECHA dissemination website (unnamed 1996)

Data for diisotridecyl adipate is not available, but an activated sludge respiratory inhibition test was conducted with the read across substance bis(2-ethylhexyl) adipate. A NOEC of 350 mg/L was determined (EC50 >350 mg/L) (unnamed 1996, available on ECHA's dissemination website https://echa.europa.eu/web/guest/information-on-chemicals/registered-substances/)

All effect levels determined are far above the water solubility of the test substances. It can be concluded that diisotridecyl adipate does not show toxic effects to STP micro-organisms within its water solubility.

7.8.4. PNEC derivation and other hazard conclusions

Table 27

PNEC DERIVATION AND OTHER HAZARD CONCLUSIONS		
Hazard assessment conclusion for the environment compartment	**Hazard conclusion**	**Remarks/Justification**
Freshwater	PNEC aqua (freshwater): 0.000016 mg/L	Assessment factor: 100 The PNEC is derived based on the NOEC of 0.0016 mg/L for Daphnia magna reported in the new OECD 211 study with DITA. Assessment factor of 100 is used as there is no chronic data adequate for PNEC derivation available on algae and fish.
Marine water	PNEC (marine waters): 0.0000016 mg/L	Assessment factor: 1000 The PNEC is derived based on the NOEC of 0.0016 mg/L for Daphnia magna reported in the new OECD 211 study with DITA. Assessment factor of 1000 is used as there is no chronic data adequate for PNEC derivation available on algae and fish.
Intermittent releases to water	PNEC (intermittent releases)>: <PNEC value> <Unit>	No PNEC derived for intermittent releases. No reliable LC/EC50 values are available for the substance.
Sediments (freshwater)	PNEC (sediment freshwater): 12.00 mg/kg (dw) derived using assessment factor) 1.80 mg/kg (dw) (derived using EPM)	Assessment factor: 1000 Extrapolation method: EPM One short-term (10 d) marine sediment toxicity test with the read across substance diisooctyl adipate is available which resulted in an 10d LC50 of >12000 mg/kg (dw), the highest concentration tested, and a 10d NOEC of 4000 mg/kg (dw). Therefore, an assessment factor of 1000 is used for the LC50 which results in a PNEC of >12.00 mg/kg (dw). In addition, as no long-term sediment toxicity data is available, the PNEC was also derived based on the aquatic PNEC and EPM (log Koc of 7.05 used as input). This resulted in a PNECsed of 3.90 mg/kg (ww) and 17.95 mg/kg (dw). As the substance is highly adsorbing (log Koc>5), the

		PECsed/PNECsed ratio derived using EPM should be increased by a factor of 10 in order to take into account the uptake via ingestion of sediment. Therefore, the PNECsed derived using EPM can be divided by 10 which results in 1.80 mg/kg (dw). This is the lowest PNEC, and thus, it is used in the risk assessment.
Sediments (marine water)	PNEC (sediment marine water): 1.20 mg/kg (dw) (derived using assessment factor) 0.18 mg/kg (dw) (derived using EPM)	Assessment factor: 10000 Extrapolation method: One short-term (10 d) marine sediment toxicity test with the read across substance diisooctyl adipate is available which resulted in a 10d LC50 of >12000 mg/kg (dw), the highest concentration tested, and a 10d NOEC of 4000 mg/kg (dw). Therefore, an assessment factor of 10000 is used for the LC50 which results in a PNEC of >1.20 mg/kg (dw). In addition, as no long-term sediment toxicity data is available, the PNEC was also derived based on the PNECaq for marine water and EPM (log Koc of 7.05 used as input). This resulted in a PNECsed of 0.39 mg/kg (ww) and 1.80 mg/kg (dw). As the substance is highly adsorbing (log Koc>5), the PECsed/PNECsed ratio derived using EPM should be increased by a factor of 10 in order to take into account the uptake via ingestion of sediment. Therefore, the PNECsed derived using EPM can be divided by 10, which results in 0.18 mg/kg (dw). This is the lowest PNEC, and thus, it is used in the risk assessment.
Sewage treatment plant	PNEC (STP): 35 mg/L	Assessment factor: 10

		An Activated Sludge Respiration Inhibition Test is available for the read across substance bi(2-ethylhexyl) adipate which resulted in a 3h NOEC of >350 mg/L. An assessment factor of 10 is used for this value.
Soil	PNEC (soil): 0.87 mg/kg (dw) (derived using assessment factor) 0.53 mg/kg (dw) (derived using EPM)	Assessment factor: 1000 Extrapolation method: EPM Two short term tests on earthworms are available for the read across substance bi(2-ethylhexyl) adipate. The lowest 14d LC50 value is 865 mg/kg (dw). Therefore, an assessment factor 1000 is applied to this value which results in a PNECsoil of 0.87 mg/kg (dw). In addition, as soil toxicity data is available only for earthworms, the PNEC soil is also derived based on the PNECaq and EPM (input values: log Koc of 7.05 and Henry's Law Constant of 44.2 Pa·m^3/mol at 12 °C). This resulted in a PNECsoil of 4,68 mg/kg (ww) and 5,31 mg/kg (dw). As the substance is highly adsorbing (log Koc>5), the PECsoil/PNECsoil ratio derived using EPM should be increased by a factor of 10 in order to take into account the uptake via ingestion of soil. Therefore, the PNECsoil derived using EPM can be divided by 10, which results in 0.53 mg/kg (dw). This is the lowest PNEC, and thus, it is used in the risk assessment.
Air	No hazard identified.	
Secondary poisoning	Not relevant.	Secondary poisoning is not considered relevant as the substance is readily biodegradable and has a low potential for bioaccumulation.

7.8.5. Conclusions for classification and labelling

Based on the available information diisotridecyl adipate is considered rapidly degradable and not bioaccumulative (BCF<500) for classification purposes.

In the acute studies with fish, aquatic invertebrates and algae nominal concentrations well above the water solubility limit of the substance were used and the concentrations were not measured. However, based on the results of the studies it seems that there are

no acute effects at the water solubility limit of the substance. Hence, the substance does not receive a classification for acute hazards.

Reliable chronic data is only available for aquatic invertebrates. The reported NOEC is 1.6 µg/L for *Daphnia magna*. It is noted that this value is above the water solubility measured in an OECD 105 for DITA (WS of 0.7 µg/L). In the long-term Daphnia test, the test solution was prepared using column elution method and the test concentration was measured to be 17.22 µg/L in the 100% eluate and 1.6 µg/L in the 10% eluate. As the substance is a UVCB and the dissolution water used in the daphnia test (purified drinking water) was different than in the OECD 105 test (deionised water), the eMSCA concluded that the test concentrations can be considered to fall in the range of water solubility of the substance. This is also supported by additional water solubility measurements reported in the registration dossier.

Based on this information, the substance receives a classification of Aquatic Chronic 1 with an M-factor of 1.

7.9. Human Health hazard assessment

The focus of the substance evaluation was on the environmental endpoints. However, the information considered to be relevant for the assessment of potential T (CMR and STOT RE), bioaccumulation potential and secondary poisoning have been considered for this assessment.

7.9.1. Toxicokinetics

Diisotridecyl adipate (DITA)

DITA is rapidly absorbed from the gastro intestinal tract and transformed by hydroxylation and conjugation reactions. Excretion of polar metabolites and conjugates may occur via urine and bile and is estimated to be substantial (Eisenbrand 2002).

Bis(2-ethylhexyl) adipate (DEHA)

The data showed that after oral administration DEHA or its metabolites are readily absorbed, and distributed to various tissues (with highest levels recovered in blood and liver).

The excretion rates were also extensive (90-100%) and rapid. After 24 hours rats and monkeys showed lower elimination in urine (60-74%) and higher elimination in faeces (app. 20 %).

Justification of use of bis(2-ethylhexyl) adipate as supporting substance for diisotridecyl adipate

DEHA and DITA have the same basic structure (diester of adipic acid) and they only differ in the chain length of the alcohol part of the esters (C 13 versus C 8) which is considered not relevant from a toxicological point of view.

7.9.2. Acute toxicity and Corrosion/Irritation

Not evaluated.

7.9.3. Sensitisation

Not evaluated.

7.9.4. Repeated dose toxicity

Not evaluated.

7.9.5. Mutagenicity

Not evaluated.

7.9.6. Carcinogenicity

Not evaluated.

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

Not evaluated.

7.9.8. Hazard assessment of physico-chemical properties

Not evaluated.

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

Not evaluated.

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

Not evaluated.

7.10. Assessment of endocrine disrupting (ED) properties

Not evaluated.

7.11. PBT and vPvB assessment

7.11.1.1. **Persistence**

Based on the most recent OECD 301F study, diisotridecyl adipate as a whole is readily biodegradable. Furthermore, in an earlier study following the same guideline and in other studies following a guideline equal or similar to OECD 301B, the degradation of the substance reached or nearly reached the pass level which supports the conclusion that the substance can degrade rapidly. Therefore, the substance as a whole does not meet the screening criteria for persistence and is not likely to meet the definitive criteria for P/vP in Annex XIII of REACH.

However, the PBT assessment has to take into account all constituents at a concentration equal or above 0.1 % (v/v). As the substance is a UVCB consisting of several isomers and some of them can be present at low concentrations, a firm conclusion on the degradation of all possible constituents cannot be made based on the tests performed with the whole substance. Therefore, BIOWIN QSAR models were performed for isomers representing the most common structures as well as theoretical worst case structures. Based on the BIOWIN predictions, isomers with higher degree of branching (at least 5 branches in total in the two sidechains) and/or with quaternary carbons may be potentially persistent. However, it is noted that taking into account the available information on the manufacturing process and analytical data on the substance, the presence of constituents with quaternary carbons is unlikely.

Furthermore, based on the BIOWIN 4 model and the biodegradation pathway predictions, primary degradation through cleavage of the ester bonds may occur leading to the formation of adipic acid and isotridecyl alcohols. Based on the available information, these degradation products are readily biodegradable.

In conclusion, most of the isomers of the substance are considered to be readily biodegradable and not meet the criteria for P/vP based on the high level of degradation observed in the ready biodegradation tests with the whole substance and the BIOWIN QSAR predictions performed for representative isomers. Some uncertainty remains regarding the degradation of isomers with higher degree of branching, and based on the available information it is not possible to firmly conclude on their persistence. However, relatively rapid primary degradation might be expected for all isomers, and the expected degradation products are not persistent. Hence, all isomers of DITA are likely to not meet the criteria for P/vP in Annex III of REACH.

7.11.1.2. **Bioaccumulation**

No experimental bioaccumulation test is available for DITA. The predicted log Kow values of the constituents are above the cut-off value of 10 suggesting limited potential for bioaccumulation and the predicted BCF values are very low. In addition, based on the high molecular size of the constituents hindered uptake and low BCF values may be expected.

Furthermore, toxicokinetic information available for the similar substance DEHA suggests that the constituents of DITA may be rapidly metabolised through cleavage of the ester bond, at least in mammals.

In conclusion, using the weight-of-evidence approach and considering the potential hindered uptake based the very high log Kow values (above 10) and molecular size as well as the low predicted BCF values and the potential rapid metabolism, the constituents of DITA are not expected to meet the criteria for B/vB in Annex XIII of REACH.

7.11.1.3. **Toxicity**

Diisotridecyl adipate is not classified as CMR or STOT RE.

In a Daphnia magna reproduction study a NOEC of 0.0016 mg/L was observed. This value is above the water solubility measured in an OECD 105 for DITA (WS of 0.7 µg/L). In the long-term Daphnia test, the test solution was prepared using column elution method and the test concentration was measured to be 17.22 µg/L in the 100% eluate and 1.6 µg/L in the 10% eluate. As the substance is a UVCB and the dissolution water used in the daphnia test (purified drinking water) was different than in the OECD 105 test (deionised water), the eMSCA concluded that the test concentrations can be considered to fall in the range of water solubility of the substance. This is also supported by additional water solubility measurements reported in the registration dossier.

In conclusion, based on the available information, DITA as a whole is considered to meet the criteria for T. There is no information on the toxicity of individual isomers of DITA.

7.11.1.4. **Overall conclusion**

Based on the available information, the constituents of diisotridecyl adipate do not meet the criteria for P/vP or B/vB but the whole substance meets the criteria for T. In conclusion, diisotridecyl adipate is not PBT/vPvB according to Annex XIII of REACH.

7.12. Exposure assessment

7.12.1. Human health

Not relevant for this assessment.

7.12.2. Environment

The main objective of this assessment is to evaluate the initial identified concerns regarding wide dispersive use, high aggregated tonnage and high RCR for the environment to check for an acceptable level of environmental exposure.

To confirm the environmentally safe use of the substance, the environmental assessment of diisotridecyl adipate has been carried out using the information provided in the registration dossier, default exposure values according to the CHESAR/EUSES models, and specific exposure scenarios provided by registrants (ATIEL, 2012).

The outcomes and results of this assessment has been calculated by the eMSCA considering the information provided by the registrants after the decision. Confidential information has been included in the Confidential Annex.

The assessed tonnage is in the range of 1,000-10,000 tonnes/year based on production and import.

The assessment performed by the eMSCA is a generic worst case assessment which covers the conditions of the individual registrants and additional information provided

(see Table 28). In order to fulfil confidentiality rules, all unpublished specific information has been included in the Confidential Annex.

The substance is a clear and yellowy organic liquid used by consumers, in articles, by professional workers (widespread uses), in formulation or re-packing, at industrial sites and in manufacturing.

Table 28

Scenario	Life-cycle stage	Description
ES0-1, ES0-2, ES0-3	Manufacture	MANUFACTURE of the substance
ES1	Formulation	FORMULATION OF LUBRICANT ADDITIVES
ES2	Formulation	HANDLING AND DILUTION OF METAL WORKING FLUID CONCENTRATES
ES3	Formulation	COMPOUNDING DRY BLENDS
ES4	Use at industrial site	INDUSTRIAL USE OF LUBRICANTS AND GREASES IN VEHICLES OR MACHINERY including filling and draining of containers and enclosed machinery and associated maintenance activities (ATIEL-ATC Group B(i)outdoor).
ES5	Use at industrial site	INDUSTRIAL USE OF LUBRICANTS AND GREASES IN OPEN SYSTEMS including application of lubricant to work pieces or equipment by dipping, brushing or spraying (without exposure to heat), e.g. mould releases, corrosion protection, slideways (ATIEL-ATC Group C(i)).
ES6	Use at industrial site	INDUSTRIAL USE OF LUBRICANTS AND GREASES IN OPEN HIGH TEMPERATURE PROCESSES e.g. quenching fluids, glass release agents (ATIEL-ATC group D(i)
ES7	Use at industrial site	INDUSTRIAL USE OF LUBRICANTS AND GREASES IN HIGH ENERGY OPEN PROCESSESS e.g. in high speed machinery such as metal rolling forming or metalworking fluids for machining and grinding (ATIEL-ATC group F(i))
ES8	Use at industrial site	GENERAL INDUSTRIAL USE OF LUBRICANTS AND GREASES IN VEHICLES OR MACHINERY. including filling and draining of containers and enclosed machinery (including engines), closed system (ATIEL- ATC Group B [i] closed system)

Scenario	Life-cycle stage	Description
ES9	Use at industrial site	COMPOUNDING PLASTISOLS
ES10	Use by professional workers	GENERAL PROFESSIONAL USE OF LUBRICANTS AND GREASES IN VEHICLES OR MACHINERY (INDOOR) including filling and draining of containers and enclosed machinery (including engines), indoor and associated maintenance activities (ATIEL-ATC Group B (p) indoor).
ES11	Use by professional workers	GENERAL PROFESSIONAL USE OF LUBRICANTS AND GREASES IN VEHICLES OR MACHINERY (OUTDOOR) including filling and draining of containers and enclosed machinery (including engines), indoor and associated maintenance activities (ATIEL-ATC Group B(p) outdoor).
ES12	Use by professional workers	PROFESSIONAL USE OF LUBRICANTS AND GREASES IN OPEN SYSTEMS (INDOOR) including application of lubricant to work pieces or equipment by dipping, brushing or spraying (without exposure to heat), e.g. mould releases, corrosion protection, slideways (ATIEL-ATC Group C(p) indoor).
ES13	Use by professional workers	PROFESSIONAL USE OF LUBRICANTS AND GREASES IN OPEN SYSTEMS (OUTDOOR) including application of lubricant to work pieces or equipment by dipping, brushing or spraying (without exposure to heat), e.g. mould releases, corrosion protection, slideways (ATIEL-ATC Group C(p) outdoor).
ES14	Use by professional workers	PROFESSIONAL USE OF LUBRICANTS AND GREASES IN HIGH ENERGY OPEN PROCESSES e.g. in high speed machinery such as metal rolling forming or metalworking fluids for machining and grinding (ATIEL-ATC Group F(p)).
ES15	Consumer use	GENERAL CONSUMER USE OF LUBRICANTS AND GREASES IN VEHICLES OR MACHINERY (ATIEL-ATC Group B(c) outdoor)

ES0-1. PRODUCTION (Company 1)

This scenario covers the production of DITA

Table. Duration, frequency and volume for Formulation.

Information type	Specific scenario	Explanation
Used amount of substance per day	*	This is based on a specific formulation volume.
Annual amount used per site	*	This is based on a specific production volume.
Emission days per site	*	Specific number of days

* This information is included in the confidential annex.

Environmental surrounding characteristics

Environmental surrounding characteristics are considered for both fresh water and marine water as follows:

Fresh water flow rate: 35,000 m^3/d (specific value),

Municipal Sewage Treatment plant discharge: $700 \cdot 10^3$ l/d (specific value).

Local freshwater dilution factor: 51

Marine water flow rate: A default dilution factor for discharges to a coastal zone (marine environment) of 100 is assumed to be representative for a realistic worst case.

Operational conditions

The following specific characteristics are considered for the production scenario

Release fraction to air from process	1E-7%
Release fraction to wastewater from process	0.0012%
Release fraction to soil from process	0.01% (EC, 2003*)
Fraction tonnage to region	100%
Fraction used at main source	100%

*Default assumptions taken from EU-TGD, 2003: Table A1.1

Since production plant is settled far away no direct emissions to the marine compartment are expected. Additionally, considering high adsorptive properties and low water solubility it is not likely that the substance reach the marine compartment form the production site.

Risk management Measures

On the table below are summarised the Risk Management measures applied and their effectivity.

Table. Risk Management Measures applied for Formulation.

Environmental compartment	Measure	Effectivity
Risk management measures (air)	Ester manufacturing process has a single release point to air from a common vacuum system serving 3 production lines. The off-gasses from the production process are treated by condensation and subsequently by water scrubbing .Losses are on average 140gVOC/hr. During DITA production 1/3 of this value could be attributed.	99%.
Risk management measures (water)	Physical/chemical separation process on the Ester plant where 60% of organic components are recovered. On-site WWTP with organic abatement of 99%	60% 99%
Risk management measures (soil)	-	Default EUSES

ES0-2. PRODUCTION (Company 2)

This scenario covers the production of DITA

Table. Duration, frequency and volume for Formulation.

Information type	Specific scenario	Explanation
Used amount of substance per day	*	This is based on a specific formulation volume.
Annual amount used per site	*	This is based on a specific production volume.
Emission days per site	*	Specific number of days

* This information included in the confidential annex.

Environmental surrounding characteristics

Environmental surrounding characteristics are considered for both fresh water and marine water as follows:

Fresh water flow rate: 84,326,400 m^3/d (specific value),

Municipal Sewage Treatment plant discharge: 74,356·10^3 l/d (specific value).

Local freshwater dilution factor: 1000

Marine water flow rate: A default dilution factor for discharges to a coastal zone (marine environment) of 100 is assumed to be representative for a realistic worst case.

Operational conditions

The following specific characteristics are considered for the production scenario

Release fraction to air from process	5E-4%
Release fraction to wastewater from process	0.110%
Release fraction to soil from process	0%
Fraction tonnage to region	100%
Fraction used at main source	100%

Since production plant is settled far away no direct emissions to the marine compartment are expected. Additionally, considering high adsorptive properties and low water solubility it is not likely that the substance reach the marine compartment form the production site.

Risk management Measures

On the table below are summarised the Risk Management measures applied and their effectivity.

Table. Risk Management Measures applied for Formulation.

Environmental compartment	Measure	Effectivity
Risk management measures (air)	Not indicated but associated to SpERC	-
Risk management measures (water)	Not indicated but associated to SpERC	-
Risk management measures (soil)	Incineration of sludge	100%

ES0-3. PRODUCTION (Company 3)

This scenario covers the production of DITA

Table. Duration, frequency and volume for Formulation.

Information type	Specific scenario	Explanation
Used amount of substance per day	*	This is based on a specific formulation volume.
Annual amount used per site	*	This is based on a specific production volume.
Emission days per site	*	Specific number of days

* This information included in the confidential annex.

Environmental surrounding characteristics

Environmental surrounding characteristics are considered for both fresh water and marine water as follows:

Fresh water flow rate: 19,800,000 m^3/d (specific value),

Municipal Sewage Treatment plant discharge: 2,604·10^4 l/d (specific value).

Local freshwater dilution factor: 761.369

Marine water flow rate: A default dilution factor for discharges to a coastal zone (marine environment) of 100 is assumed to be representative for a realistic worst case.

Operational conditions

The following specific characteristics are considered for the production scenario

Release fraction to air from process	0.00005%
Release fraction to wastewater from process	2.E-11%
Release fraction to soil from process	0%
Fraction tonnage to region	100%
Fraction used at main source	100%

Risk management Measures

On the table below are summarised the Risk Management measures applied and their effectivity.

Table. Risk Management Measures applied for Formulation.

Environmental compartment	Measure	Effectivity
Risk management measures (air)	Not indicated but associated to SpERC	-
Risk management measures (water)	Not indicated but associated to SpERC	-
Risk management measures (soil)	-	100%

Since production plant is settled far away no direct emissions to the marine compartment are expected. Additionally, considering high adsorptive properties and low water solubility it is not likely that the substance reach the marine compartment form the production site.

ES1. INDUSTRIAL FORMULATION of lubricant additives - (ERC2 – Formulation of preparations)

This scenario covers the industrial formulation of lubricants additives, lubricants and greases (ATIEL-ATC Group A(i)outdoor).

The SpERC ATIEL ATC SpERC 2.A(i) (2012) has been applied base on sector specific knowledge.

Table. Duration, frequency and volume for Formulation.

Information type	Generic scenario	Explanation
Used amount of substance per day	*	This is based on a generic formulation volume.
Annual amount used per site	*	This is based on a generic formulation volume.
Emission days per site	*	Specific number of days

* This information included in the confidential annex.

Environmental surrounding characteristics

Environmental surrounding characteristics are considered for both fresh water and marine water as follows:

Fresh water flow rate: 18,000 m^3/d (default value),

Municipal Sewage Treatment plant discharge: $2 \cdot 10^3$ m^3/d (default value).

Marine water flow rate: A default dilution factor for discharges to a coastal zone (marine environment) of 100 is assumed to be representative for a realistic worst case.

STP considered

Operational conditions

The following specific characteristics are considered for the ATIEL ATC SpERC 2.A(i)

Release fraction to air from process	0.00005%
Release fraction to wastewater from process	2E-11%
Release fraction to soil from process	0%
Fraction tonnage to region	100%
Fraction used at main source	100%

According to ATIEL ATC SpERC 2.A(i) there is no emissions to soil since based on a survey biosolids of industrial origin are incinerated.

Based on sector knowledge information and responses to the ATIEL-ATC questionnaire 2010 Release estimations to air are based on emission data for VOC and hydrocarbons.

Negligible wastewater emissions as process operates without water contact

Risk management Measures

On the table below are summarised the Risk Management measures applied and their effectivity.

Table. Risk Management Measures applied for Formulation.

Environmental compartment	Measure	Effectivity
Risk management measures (air)	Wet scrubber - for gas removal, or b) Waste gas treatment - thermal oxidation#	99%
Risk management measures (water)	User sites are assumed to be provided with oil/water separators or equivalent and for waste water to be discharged via public sewer system	90-95%
Risk management measures	No emissions to soil since based on a	100%

(soil)	survey biosolids of industrial origin are incinerated.	

ES2. USES AT INDUSTRIAL SITE (ERC2 - Formulation of preparations)

This scenario covers the industrial handling and dilution of metal working fluid concentrates (ATIEL-ATC Group E(i)).

The SpERC ATIEL-ATC SPERC 2.Ei.v1 (2012) has been applied base on sector specific knowledge.

Table. Duration, frequency and volume for Formulation.

Information type	Generic scenario	Explanation
Used amount of substance per day	*	This is based on a generic formulation volume.
Annual amount used per site	*	This is based on a generic formulation volume.
Emission days per site	*	Specific number of days

* This information included in the confidential annex.

Environmental surrounding characteristics

Environmental surrounding characteristics are considered for both fresh water and marine water as follows:

Fresh water flow rate: 18,000 m^3/d (default value),

Municipal Sewage Treatment plant discharge: $2 \cdot 10^3$ m^3/d (default value).

Marine water flow rate: A default dilution factor for discharges to a coastal zone (marine environment) of 100 is assumed to be representative for a realistic worst case.

STP considered

Operational conditions

The following specific characteristics are considered for the ATIEL-ATC SPERC 2.Ei.v1

Release fraction to air from process	0.00005%
Release fraction to wastewater from process	2E-11%
Release fraction to soil from process	0%
Fraction tonnage to region	100%
Fraction used at main source	100%

According to ATIEL ATC SpERC 2.A(i) there is no emissions to soil since based on a survey biosolids of industrial origin are incinerated.

Based on sector knowledge information and responses to the ATIEL-ATC questionnaire 2010 Release estimations to air are based on emission data for VOC and hydrocarbons.

Negligible wastewater emissions as process operates without water contact

Risk management Measures

On the table below are summarised the Risk Management measures applied and their effectivity.

Table. Risk Management Measures applied for Formulation.

Environmental compartment	Measure	Effectivity
Risk management measures (air)	Wet scrubber - for gas removal, or b) Waste gas treatment - thermal oxidation#	99%
Risk management measures (water)	User sites are assumed to be provided with oil/water separators or equivalent and for waste water to be discharged via public sewer system	90-95%
Risk management measures (soil)	No emissions to soil since based on a survey biosolids of industrial origin are incinerated.	100%

ES3. FORMULATION - COMPOUNDING DRY BLENDS – (ERC3 - Formulation in articles)

This scenario covers the compounding dry blends.

Table. Duration, frequency and volume for Formulation.

Information type	Generic scenario	Explanation
Used amount of substance per day	*	This is based on a generic formulation volume.
Annual amount used per site	*	This is based on a generic formulation volume.
Emission days per site	*	Specific number of days

* This information included in the confidential annex.

Environmental surrounding characteristics

Environmental surrounding characteristics are considered for both fresh water and marine water as follows:

Fresh water flow rate: 18,000 m^3/d (default value),

Municipal Sewage Treatment plant discharge: $2 \cdot 10^3$ m^3/d (default value).

Marine water flow rate: A default dilution factor for discharges to a coastal zone (marine environment) of 100 is assumed to be representative for a realistic worst case.

STP considered.

Operational conditions

The following characteristics are considered:

Release fraction to air from process	0.005%
Release fraction to wastewater from process	0.005%
Release fraction to soil from process	0.001%
Fraction tonnage to region	100%
Fraction used at main source	100%

Risk management Measures

No specific RMMs applied.

ES4. INDUSTRIAL USE AT SITE – (ERC4 – industrial use of processing aids)

This scenario covers the industrial use of lubricants and greases in vehicles or machinery, including filling and draining of containers and enclosed machinery and associated maintenance activities (ATIEL-ATC Group B(i)outdoor).

The SpERC ATIEL-ATC SPERC 4.Bi.v1 (2012) has been applied base on sector specific knowledge.

Table. Duration, frequency and volume for Formulation.

Information type	Generic scenario	Explanation
Used amount of substance per day	*	This is based on a generic formulation volume.
Annual amount used per site	*	This is based on a generic formulation volume.
Emission days per site	*	Specific number of days

* This information included in the confidential annex.

Environmental surrounding characteristics

Environmental surrounding characteristics are considered for both fresh water and marine water as follows:

Fresh water flow rate: 18,000 m^3/d (default value),

Municipal Sewage Treatment plant discharge: $2 \cdot 10^3$ m^3/d (default value).

Marine water flow rate: A default dilution factor for discharges to a coastal zone (marine environment) of 100 is assumed to be representative for a realistic worst case.

STP considered.

Operational conditions

The following specific characteristics are considered for the ATIEL-ATC SPERC 4.Bi.v1

Release fraction to air from process	0.00005%
Release fraction to wastewater from process	2E-11%
Release fraction to soil from process	0%
Fraction tonnage to region	100%
Fraction used at main source	100%

According to ATIEL-ATC SPERC 4.Bi.v1 there is no emissions to soil since based on a survey biosolids of industrial origin are incinerated.

Based on sector knowledge information and responses to the ATIEL-ATC questionnaire 2010 Release estimations to air are based on emission data for VOC and hydrocarbons.

Negligible wastewater emissions as process operates without water contact.

Risk management Measures

On the table below are summarised the Risk Management measures applied and their effectivity.

Table. Risk Management Measures applied for Formulation.

Environmental compartment	Measure	Effectivity
Risk management measures (air)	Wet scrubber - for gas removal, or b) Waste gas treatment - thermal oxidation#	99%
Risk management measures (water)	User sites are assumed to be provided with oil/water separators or equivalent and for waste water to be discharged via public sewer system	90-95%
Risk management measures (soil)	No emissions to soil since based on a survey biosolids of industrial origin are incinerated.	100%

ES5. INDUSTRIAL USE IN OPEN SYSTEM – (ERC4 – industrial use of processing aids)

This scenario covers the industrial use of lubricants and greases in open systems, including application of lubricant to work pieces or equipment by dipping, brushing or spraying (without exposure to heat), e.g. mould releases, corrosion protection, slideways. Includes associated product storage, material transfers, sampling and maintenance activities (ATIEL-ATC Group C(i)).

The SpERC ATIEL-ATC SPERC 4.Ci.v1 (2012) has been applied base on sector specific knowledge.

Table. Duration, frequency and volume for Formulation.

Information type	Generic scenario	Explanation
Used amount of substance per day	*	This is based on a generic formulation volume.
Annual amount used per site	*	This is based on a generic formulation volume.
Emission days per site	*	Specific number of days

* This information included in the confidential annex.

Environmental surrounding characteristics

Environmental surrounding characteristics are considered for both fresh water and marine water as follows:

Fresh water flow rate: 18,000 m^3/d (default value),

Municipal Sewage Treatment plant discharge: $2 \cdot 10^3$ m^3/d (default value).

Marine water flow rate: A default dilution factor for discharges to a coastal zone (marine environment) of 100 is assumed to be representative for a realistic worst case.

STP considered

Operational conditions

The following specific characteristics are considered for the ATIEL-ATC SPERC 4.Ci.v1

Release fraction to air from process	0.00005%
Release fraction to wastewater from process	2E-11%
Release fraction to soil from process	0%
Fraction tonnage to region	100%
Fraction used at main source	100%

According to ATIEL-ATC SPERC 4.Ci.v1 there is no emissions to soil since based on a survey biosolids of industrial origin are incinerated.

Based on sector knowledge information and responses to the ATIEL-ATC questionnaire 2010 Release estimations to air are based on emission data for VOC and hydrocarbons.

Negligible wastewater emissions as process operates without water contact.

Risk management Measures

On the table below are summarised the Risk Management measures applied and their effectivity.

Table. Risk Management Measures applied for Formulation.

Environmental compartment	Measure	Effectivity
Risk management measures (air)	Wet scrubber - for gas removal, or b) Waste gas treatment - thermal oxidation#	99%
Risk management measures (water)	User sites are assumed to be provided with oil/water separators or equivalent and for waste water to be discharged via public sewer system	90-95%
Risk management measures (soil)	No emissions to soil since based on a survey biosolids of industrial origin are incinerated.	100%

ES6. INDUSTRIAL USE IN OPEN HIGH TEMPERATURE PROCESSES – (ERC4 – industrial use of processing aids)

This scenario covers the industrial use of lubricants and greases in open high temperature processes, e.g. quenching fluids, glass release agents (ATIEL-ATC group D(i) - DITA.

The ATIEL-ATC Di – DITA (is taken from the SpERC factsheet Ci) has been applied base on sector specific knowledge.

Table. Duration, frequency and volume for Formulation.

Information type	Generic scenario	Explanation
Used amount of substance per day	*	This is based on a generic formulation volume.
Annual amount used per site	*	This is based on a generic formulation volume.
Emission days per site	*	Specific number of days

* This information included in the confidential annex.

Environmental surrounding characteristics

Environmental surrounding characteristics are considered for both fresh water and marine water as follows:

Fresh water flow rate: 18,000 m^3/d (default value),

Municipal Sewage Treatment plant discharge: $2 \cdot 10^3$ m^3/d (default value).

Marine water flow rate: A default dilution factor for discharges to a coastal zone (marine environment) of 100 is assumed to be representative for a realistic worst case.

STP considered

Operational conditions

The following specific characteristics are considered for the ATIEL-ATC Di

Release fraction to air from process	0.005%
Release fraction to wastewater from process	2E-10%
Release fraction to soil from process	0%
Fraction tonnage to region	100%
Fraction used at main source	100%

Risk management Measures

No information on the RMMs.

ES7. INDUSTRIAL USE OF LUBRICANTS IN HIGH ENERGY OPEN PROCESSESS – (ERC4 – industrial use of processing aids)

This scenario covers the industrial use of lubricants and greases in high energy open processes, e.g. in high speed machinery such as metal rolling forming or metalworking fluids for machining and grinding (ATIEL-ATC group F(i)).

The SpERC ATIEL-ATC SPERC 4.Fi.v1 (2012) has been applied base on sector specific knowledge.

Table. Duration, frequency and volume for Formulation.

Information type	Generic scenario	Explanation
Used amount of substance per day	*	This is based on a generic formulation volume.
Annual amount used per site	*	This is based on a generic formulation volume.
Emission days per site	*	Specific number of days

* This information included in the confidential annex.

Environmental surrounding characteristics

Environmental surrounding characteristics are considered for both fresh water and marine water as follows:

Fresh water flow rate: 18,000 m^3/d (default value),

Municipal Sewage Treatment plant discharge: $2 \cdot 10^3$ m^3/d (default value).

Marine water flow rate: A default dilution factor for discharges to a coastal zone (marine environment) of 100 is assumed to be representative for a realistic worst case.

STP considered

Operational conditions

The following specific characteristics are considered for the ATIEL-ATC SPERC 4.Fi.v1

Release fraction to air from process	0.00005%
Release fraction to wastewater from process	2E-11%
Release fraction to soil from process	0%
Fraction tonnage to region	100%
Fraction used at main source	100%

According to ATIEL-ATC SPERC 4.Fi.v1 there is no emissions to soil since based on a survey biosolids of industrial origin are incinerated.

Based on sector knowledge information and responses to the ATIEL-ATC questionnaire 2010 Release estimations to air are based on emission data for VOC and hydrocarbons.

Negligible wastewater emissions as process operates without water contact.

Risk management Measures

On the table below are summarised the Risk Management measures applied and their effectivity.

Table. Risk Management Measures applied for Formulation.

Environmental compartment	Measure	Effectivity
Risk management measures (air)	Wet scrubber - for gas removal, or b) Waste gas treatment - thermal oxidation#	99%
Risk management measures (water)	User sites are assumed to be provided with oil/water separators or equivalent and for waste water to be discharged via public sewer system	90-95%
Risk management measures (soil)	No emissions to soil since based on a survey biosolids of industrial origin are incinerated.	100%

ES8. INDUSTRIAL USE OF LUBRICANTS IN HIGH ENERGY OPEN PROCESSESS – (ERC7 – industrial use of substances in closed systems)

This scenario covers the industrial use of lubricants and greases in vehicles or machinery. Includes filling and draining of containers and enclosed machinery)(including engines), closed systems (ATIEL-ATC Group B(i) closed systems)

The SpERC ATIEL-ATC SPERC 7.Bi – DITA is taken from the SPERC factsheet Bi released by ATIEL (2012).

Table. Duration, frequency and volume for Formulation.

Information type	Generic scenario	Explanation
Used amount of substance per day	*	This is based on a generic formulation volume.
Annual amount used per site	*	This is based on a generic formulation volume.
Emission days per site	*	Specific number of days

* This information included in the confidential annex.

Environmental surrounding characteristics

Environmental surrounding characteristics are considered for both fresh water and marine water as follows:

Fresh water flow rate: 18,000 m^3/d (default value),

Municipal Sewage Treatment plant discharge: $2 \cdot 10^3$ m^3/d (default value).

Marine water flow rate: A default dilution factor for discharges to a coastal zone (marine environment) of 100 is assumed to be representative for a realistic worst case.

STP considered

Operational conditions

The following specific characteristics are considered for the ATIEL-ATC SPERC 4.Fi.v1

Release fraction to air from process	0.00005%
Release fraction to wastewater from process	2E-11%
Release fraction to soil from process	0%
Fraction tonnage to region	100%
Fraction used at main source	100%

According to ATIEL-ATC SPERC 4.Fi.v1 there is no emissions to soil since based on a survey biosolids of industrial origin are incinerated.

Based on sector knowledge information and responses to the ATIEL-ATC questionnaire 2010 Release estimations to air are based on emission data for VOC and hydrocarbons.

Negligible wastewater emissions as process operates without water contact.

Risk management Measures

On the table below are summarised the Risk Management measures applied and their effectivity.

Table. Risk Management Measures applied for Formulation.

Environmental compartment	Measure	Effectivity
Risk management measures (air)	Wet scrubber - for gas removal, or b) Waste gas treatment - thermal oxidation#	99%
Risk management measures (water)	User sites are assumed to be provided with oil/water separators or equivalent and for waste water to be discharged via public sewer system	90-95%
Risk management measures (soil)	No emissions to soil since based on a survey biosolids of industrial origin are incinerated.	100%

ES9. COMPOUNDING PLASTISOLS – (ERC5 – industrial use resulting in inclusion into or onto a matrix)

Table. Duration, frequency and volume for Formulation.

Information type	Generic scenario	Explanation
Used amount of substance per day	*	This is based on a generic formulation volume.
Annual amount used per site	*	This is based on a generic formulation volume.
Emission days per site	*	Specific number of days

* This information included in the confidential annex.

Environmental surrounding characteristics

Environmental surrounding characteristics are considered for both fresh water and marine water as follows:

Fresh water flow rate: 18,000 m^3/d (default value),

Municipal Sewage Treatment plant discharge: $2 \cdot 10^3$ m^3/d (default value).

Marine water flow rate: A default dilution factor for discharges to a coastal zone (marine environment) of 100 is assumed to be representative for a realistic worst case.

STP considered

Operational conditions

The following specific characteristics are considered for the ATIEL-ATC SPERC 4.Fi.v1

Release fraction to air from process	0.00005%
Release fraction to wastewater from process	0.0005%
Release fraction to soil from process	0.0001%
Fraction tonnage to region	10%
Fraction used at main source	100%

Risk management Measures

No information on the RMMs.

ES10. GENERAL PROFESSIONAL USE OF LUBRICANTS AND GREASES IN VEHICLES OR MACHINERY – (ERC9a – Wide dispersive indoor use of substances in closed systems)

This scenario covers the general use of lubricants and greases in vehicles or machinery. Includes filling and draining of containers and enclosed machinery (including engines), indoor and associated maintenance activities (ATIEL-ATC Group B (p) indoor).

The SpERC ATIEL-ATC SPERC 9.Bp.v1 1 (2012) has been applied base on sector specific knowledge and the OECD Emission Scenario Document on Lubricants and Lubricants Additives, Nº10 (OECD, 2004).

Table. Duration, frequency and volume for Formulation.

Information type	Generic scenario	Explanation
Used amount of substance per day	*	This is based on a generic formulation volume.
Annual amount used per site	*	This is based on a generic formulation volume.
Emission days per site	*	Specific number of days

* This information included in the confidential annex.

Environmental surrounding characteristics

Environmental surrounding characteristics are considered for both fresh water and marine water as follows:

Fresh water flow rate: 18,000 m^3/d (default value),

Municipal Sewage Treatment plant discharge: $2 \cdot 10^3$ m^3/d (default value).

Marine water flow rate: A default dilution factor for discharges to a coastal zone (marine environment) of 100 is assumed to be representative for a realistic worst case.

STP considered

Operational conditions

The following specific characteristics are considered for the ATIEL-ATC SPERC 9.Bp.v1

Release fraction to air from process	0.0005% (EC, 2003*)
Release fraction to wastewater from process	0.0005% (EC, 2003*)
Release fraction to soil from process	0.001% (EC, 2003*)
Fraction tonnage to region	10%
Fraction used at main source	0.2%

*Default assumptions taken from EU-TGD, 2003: Table A3.8

Negligible wastewater emissions as process operates without water contact.

Risk management Measures

On the table below are summarised the Risk Management measures applied and their effectivity.

Table. Risk Management Measures applied for Formulation.

Environmental compartment	Measure	Effectivity
Risk management measures (air)	None	EUSES default
Risk management measures (water)	Waste water is assumed to be discharged via public sewer system.	EUSES default
Risk management measures (soil)	None	EUSES default

ES11. GENERAL PROFESSIONAL USE OF LUBRICANTS AND GREASES IN VEHICLES OR MACHINERY – (ERC9b – Wide dispersive outdoor use of substances in closed systems)

This scenario covers the general use of lubricants and greases in vehicles or machinery. Includes filling and draining of containers and enclosed machinery (including engines), indoor and associated maintenance activities (ATIEL-ATC Group B(p) outdoor).

The SpERC ATIEL-ATC SPERC 9.Bp.v1 1 (2012) has been applied base on sector specific knowledge and the OECD Emission Scenario Document on Lubricants and Lubricants Additives, Nº10 (OECD, 2004).

Table. Duration, frequency and volume for Formulation.

Information type	Generic scenario	Explanation
Used amount of substance per day	*	This is based on a generic formulation volume.
Annual amount used per site	*	This is based on a generic formulation volume.
Emission days per site	*	Specific number of days

* This information included in the confidential annex.

Environmental surrounding characteristics

Environmental surrounding characteristics are considered for both fresh water and marine water as follows:

Fresh water flow rate: 18,000 m^3/d (default value),

Municipal Sewage Treatment plant discharge: $2 \cdot 10^3$ m^3/d (default value).

Marine water flow rate: A default dilution factor for discharges to a coastal zone (marine environment) of 100 is assumed to be representative for a realistic worst case.

No STP is considered

Operational conditions

The following specific characteristics are considered for the ATIEL-ATC SPERC 9.Bp.v1

Release fraction to air from process	0.0005% (EC, 2003*)
Release fraction to wastewater from process	0.0005% (EC, 2003*)
Release fraction to soil from process	0.001% (EC, 2003*)
Fraction tonnage to region	10%
Fraction used at main source	0.2%

*Default assumptions taken from EU-TGD, 2003: Table A3.8

Negligible wastewater emissions as process operates without water contact.

Risk management Measures

On the table below are summarised the Risk Management measures applied and their effectivity.

Table. Risk Management Measures applied for Formulation.

Environmental compartment	Measure	Effectivity
Risk management measures (air)	None	EUSES default
Risk management measures (water)	Waste water is assumed to be discharged via public sewer system.	EUSES default
Risk management measures (soil)	None	EUSES default

ES12. PROFESSIONAL USE IN OPEN SYSTEMS – (ERC8A – Wide dispersive indoor use of processing aids in open systems)

This scenario covers professional use of lubricants and greases in open systems, including application of lubricant to work pieces or equipment by dipping, brushing or spraying (without exposure to heat), e.g. mould releases, corrosion protection, slideways. Includes associated product storage, material transfers, sampling and maintenance activities (ATIEL-ATC Group C(p) indoor).

The SpERC ATIEL-ATC SPERC 8.Cp.v1 – DITA (2013) has been applied base on sector specific knowledge.

Table. Duration, frequency and volume for Formulation.

Information type	Generic scenario	Explanation
Used amount of substance per day	*	This is based on a generic formulation volume.
Annual amount used per site	*	This is based on a generic formulation volume.
Emission days per site	*	Specific number of days

* This information included in the confidential annex.

Environmental surrounding characteristics

Environmental surrounding characteristics are considered for both fresh water and marine water as follows:

Fresh water flow rate: 18,000 m^3/d (default value),

Municipal Sewage Treatment plant discharge: $2 \cdot 10^3$ m^3/d (default value).

Marine water flow rate: A default dilution factor for discharges to a coastal zone (marine environment) of 100 is assumed to be representative for a realistic worst case.

STP considered

Operational conditions

The following specific characteristics are considered for the ATIEL-ATC SPERC 8.Cp.v1 - DITA

Release fraction to air from process	0.0005% (EC, 2003*)
Release fraction to wastewater from process	0.0005% (EC, 2003*)
Release fraction to soil from process	0.001% (EC, 2003*)
Fraction tonnage to region	10%
Fraction used at main source	0.2%

*Default assumptions taken from EU-TGD, 2003: Table A3.8

Negligible wastewater emissions as process operates without water contact

Risk management Measures

On the table below are summarised the Risk Management measures applied and their effectivity.

Table. Risk Management Measures applied for Formulation.

Environmental compartment	Measure	Effectivity
Risk management measures (air)	None	EUSES default
Risk management measures (water)	Waste water is assumed to be discharged via public sewer system.	EUSES default
Risk management measures (soil)	None	EUSES default

ES13. PROFESSIONAL USE IN OPEN SYSTEMS – (ERC8d – Wide dispersive outdoor use of processing aids in open systems)

This scenario covers professional use of lubricants and greases in open systems, including application of lubricant to work pieces or equipment by dipping, brushing or spraying (without exposure to heat), e.g. mould releases, corrosion protection, slideways. Includes associated product storage, material transfers, sampling and maintenance activities (ATIEL-ATC Group C(p) outdoor).

The SpERC ATIEL-ATC SPERC 8.Cp.v1 – DITA (2013) has been applied base on sector specific knowledge.

Table. Duration, frequency and volume for Formulation.

Information type	Generic scenario	Explanation
Used amount of substance per day	*	This is based on a generic formulation volume.
Annual amount used per site	*	This is based on a generic formulation volume.
Emission days per site	*	Specific number of days

* This information included in the confidential annex.

Environmental surrounding characteristics

Environmental surrounding characteristics are considered for both fresh water and marine water as follows:

Fresh water flow rate: 18,000 m^3/d (default value),

Municipal Sewage Treatment plant discharge: $2 \cdot 10^3$ m^3/d (default value).

Marine water flow rate: A default dilution factor for discharges to a coastal zone (marine environment) of 100 is assumed to be representative for a realistic worst case.

No STP is considered

Operational conditions

The following specific characteristics are considered for the ATIEL-ATC SPERC 8.Cp.v1 - DITA

Release fraction to air from process	0.0005% (EC, 2003*)
Release fraction to wastewater from process	0.0005% (EC, 2003*)
Release fraction to soil from process	0.001% (EC, 2003*)
Fraction tonnage to region	10%
Fraction used at main source	0.2%

*Default assumptions taken from EU-TGD, 2003: Table A3.8

Negligible wastewater emissions as process operates without water contact

Risk management Measures

On the table below are summarised the Risk Management measures applied and their effectivity.

Table. Risk Management Measures applied for Formulation.

Environmental compartment	Measure	Effectivity
Risk management measures (air)	None	EUSES default
Risk management measures (water)	Waste water is assumed to be discharged via public sewer system.	EUSES default
Risk management measures (soil)	None	EUSES default

ES14. PROFESSIONAL USE OF LUBIRCANTS IN HIGH ENERGY OPEN PROCESSES – (ERC8A – Wide dispersive indoor use of processing aids in open systems)

This scenario covers the professional use of lubricants in high energy open processes, e.g. in high speed machinery such as metal rolling forming or metalworking fluids for machining and grinding (ATIEL-ATC Group F(p)).

The SpERC ATIEL-ATC SPERC 8.Fp.v1 – DITA (2012) has been applied base on sector specific knowledge.

Table. Duration, frequency and volume for Formulation.

Information type	Generic scenario	Explanation
Used amount of substance per day	*	This is based on a generic formulation volume.
Annual amount used per site	*	This is based on a generic formulation volume.
Emission days per site	*	Specific number of days

* This information included in the confidential annex.

Environmental surrounding characteristics

Environmental surrounding characteristics are considered for both fresh water and marine water as follows:

Fresh water flow rate: 18,000 m^3/d (default value),

Municipal Sewage Treatment plant discharge: $2 \cdot 10^3$ m^3/d (default value).

Marine water flow rate: A default dilution factor for discharges to a coastal zone (marine environment) of 100 is assumed to be representative for a realistic worst case.

STP is considered

Operational conditions

The following specific characteristics are considered for the ATIEL-ATC SPERC 8.Fp.v1 - DITA

Release fraction to air from process	0.0005% (EC, 2003*)
Release fraction to wastewater from process	0.001%
Release fraction to soil from process	0.001% (EC, 2003*)
Fraction tonnage to region	10%
Fraction used at main source	100%

*Default assumptions taken from EU-TGD, 2003: Table A3.8

Negligible wastewater emissions as process operates without water contact.

Risk management Measures

On the table below are summarised the Risk Management measures applied and their effectivity.

Table. Risk Management Measures applied for Formulation.

Environmental compartment	Measure	Effectivity
Risk management measures (air)	None	EUSES default
Risk management measures (water)	Waste water is assumed to be discharged via public sewer system.	EUSES default
Risk management measures (soil)	None	EUSES default

ES15. GENERAL CONSUMER USE OF LUBRICANTS AND GREASES IN VEHICLES OR MACHINERY – (ERC9B – Wide dispersive outdoor use of substances in closed systems)

This scenario covers consumer use of lubricants and greases in vehicles or machinery. Includes filling and draining of containers and enclosed machinery (including engines) and associated maintenance activities (ATIEL-ATC Group B(c) outdoor).

The SpERC ATIEL-ATC SPERC 9.Bc.v1 – DITA (2012) has been applied base on sector specific knowledge.

Table. Duration, frequency and volume for Formulation.

Information type	Generic scenario	Explanation
Used amount of substance per day	*	This is based on a generic formulation volume.
Annual amount used per site	*	This is based on a generic formulation volume.
Emission days per site	*	Specific number of days

* This information included in the confidential annex.

Environmental surrounding characteristics

Environmental surrounding characteristics are considered for both fresh water and marine water as follows:

Fresh water flow rate: 18,000 m^3/d (default value),

Municipal Sewage Treatment plant discharge: $2 \cdot 10^3$ m^3/d (default value).

Marine water flow rate: A default dilution factor for discharges to a coastal zone (marine environment) of 100 is assumed to be representative for a realistic worst case.

No STP is considered

Operational conditions

The following specific characteristics are considered for the ATIEL-ATC SPERC 9.Bc.v1

- DITA

Release fraction to air from process	0.005%
Release fraction to wastewater from process	0.0005%
Release fraction to soil from process	0.0001%
Fraction tonnage to region	10%
Fraction used at main source	0.2%

Risk management Measures

On the table below are summarised the Risk Management measures applied and their effectivity.

Table. Risk Management Measures applied for Formulation.

Environmental compartment	Measure	Effectivity
Risk management measures (air)	None	EUSES default
Risk management measures (water)	Waste water is assumed to be discharged via public sewer system.	EUSES default
Risk management measures (soil)	None	EUSES default

7.12.2.1. **Aquatic compartment (incl. sediment)**

According to the new available information on exposure and risk management measures, the following PECs have been calculated by the eMSCA for the aquatic compartment.

Table 29. PECs for the aquatic compartment

Scenario	Freshwater (mg/L)	Freshwater Sed. (mg/kg dw)	Marine water (mg/L)	Marine sediment (mg/kg dw)
ES0-1	1.12E-06	1.47	7.12E-6	9.32
ES0-2	1.71E-07	0.224	2.36E-05	30.8
ES0-3	2.49E-08	0.0326	2.1E-06	2.75
ES1	7.61E-09	9.96E-3	1.79E-9	2.35E-3
ES2	7.61E-9	9.96E-3	1.79E-9	2.35E-3
ES3	1.1E-6	1.44	1.37E-6	1.79
ES4	7.61E-9	9.96E-3	1.79E-9	2.35E-3
ES5	7.61E-9	9.96E-3	1.79E-9	2.35E-3
ES6	7.61E-9	9.96E-3	1.79E-9	2.35E-3
ES7	7.61E-9	9.96E-3	1.79E-9	2.35E-3
ES8	7.61E-9	9.96E-3	1.79E-9	2.35E-3
ES9	4.44E-7	0.581	5.49E-7	0.719
ES10	5.62E-7	0.736	5.97E-7	0.912
ES11	6.26E-7	0.82	7.77E-7	1.02
ES12	5.61E-7	0.734	6.95E-7	0.911
ES13	5.63E-7	0.738	6.99E-7	0.915
ES14	5.58E-7	0.731	6.97E-7	0.913
ES15	7.73E-9	0.010	1.94E-9	2.55E-3

7.12.2.2. **Terrestrial compartment**

According to the information on exposure provided by registrants, the following local PECs are calculated by the eMSCA for the terrestrial compartment.

Table 30. PECs for the terrestrial compartment

Scenario	Agricultural soil (mg/kg dw)
ES0-1	2.2
ES0-2	7.29
ES0-3	0.651
ES1	6.84E-04
ES2	6.30E-04
ES3	0.424
ES4	6.84E-04
ES5	6.84E-04
ES6	7.16E-03
ES7	6.84E-04
ES8	6.85E-04
ES9	0.17
ES10	0.216
ES11	0.241
ES12	0.215
ES13	0.216
ES14	2.15
ES15	6.65E-04

7.12.2.3. **Atmospheric compartment**

Not relevant for the assessment.

7.13. Risk characterisation

Initial grounds of concern regarding RCRs > 1 for some of the registrants have been removed. Estimated RCRs are included in the next table.

Table 31. RCRs calculated by the eMSCA for the aquatic and terrestrial compartment.

Scenario	Freshwater	Freshwater Sed.	Marine water	Marine sediment	Soil
ES0-1	0.07	0.7	4.45	3.88	2.55
ES0-2	0.01	0.107	14.7	12.9	8.43
ES0-3	1.55E-03	0.015	1.31	1.15	0.752
ES1	4.75E-04	4.75E-03	1.12E-03	9.79E-04	7.91E-04
ES2	4.75E-04	4.75E-03	1.12E-03	9.79E-04	7.28E-04
ES3	0.0687	0.687	0.856	0.748	7.91E-04
ES4	4.75E-04	4.75E-03	1.12E-03	9.79E-04	7.91E-04
ES5	4.75E-04	4.75E-03	1.12E-03	9.79E-04	7.91E-04
ES6	4.75E-04	4.75E-03	1.12E-03	9.79E-04	8.28E-03
ES7	4.75E-04	4.75E-03	1.12E-03	9.79E-04	7.91E-04
ES8	4.75E-04	4.75E-03	1.12E-03	9.79E-04	7.91E-04
ES9	0.0277	0.277	0.343	0.3	0.197
ES10	0.0351	0.351	0.435	0.38	0.25
ES11	0.0391	0.391	0.486	0.424	0.278
ES12	0.035	0.35	0.435	0.38	0.249
ES13	0.437	0.352	0.437	0.381	0.25
ES14	4.83E-4	0.349	0.436	0.38	0.218
ES15	4.75E-4	9.51E-03	1.12E-03	3.92E-3	7.69E-04

The assessment results in RCS >1 for the marine and terrestrial compartments regarding the production sites. However, these results can be minimised considering that production plants are located far away from sea and therefore no direct emissions to the marine compartment are expected. Additionally, considering high adsorptive properties and low water solubility it is not likely that the substance would reach the marine compartment from the production sites.

Regarding soil, production sites indicate incineration of sludge, and therefore no exposure is expected. Registrants should check that sludge incineration is performed for their production sites.

Therefore, after the consideration of the exposure refinement carried out by the eMSCA it was concluded that there is no need for further actions or risk management measures to be implemented. Registrants should revise their risk assessment in case of any change of circumstances, such as relocation of production sites close to the sea or stopping sludge incineration.

7.14. References

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7.15. Abbreviations

ASTM	American Society for Testing and Materials
B/vB	Bioaccumulative/very Bioaccumulative
BCF	Bioconcentration factor
C&L	Classification & Labelling
CMR	Carcinogenic, Mutagenic or Toxic to Reproduction
CO_2	Carbon dioxide
CoRAP	The Community rolling action plan
DITA	diisotridecyl adipate
DEHA	bis (2- ethylhexyl) adipate
DEPT CNMR	Distortionless Enhancement of Polarisation Transfer – Carbon Nuclear Magnetic Resonance
dw	dry weight
EAWAG	Swiss Federal Institute of Aquatic Science and Technology (Eidgeno¨ssische Anstalt fu¨r Wasserversorgung, Abwasserreinigung und Gewa¨sserschutz)
EC10	Effective Concentration, 10%
EC50	Median Effective Concentration
ECHA	European Chemicals Agency
EL50	Median Effective Loading rate
eMSCA	evaluating Member State Compentent Authority
EPM	Equilibrium Partitioning Method
ES	Exposure Scenario
GI	Gastrointestinal
GLP	Good Laboratory Practice
HLC	Henry´s Law Constants
Koa	Octanol-air partition coefficient
Koc	Organic carbon normalised adsorption coefficient
Kow	Octanol / water partition coefficient
LC50	Median Lethal Concentration
LL50	Median Lethal Loading rate
LOEC	Lowest Observed Effect Concentration
LOQ	Limit of Quantification
MCI	Molecular Connectivity Index
NOEC	No Observed Effect Concentration
NOELR	No Observed Effect Loading Rate
O_2	Oxygen
OECD	Organisation for Economic Co-operation and Development
P/vP	Persistent/very Persistent
PBT	Persistent, Bioaccumulative and Toxic
PEC	Predicted Environmental Concentration

PNEC	Predicted No Effect Concentration
QSAR	Quantitative Structure–Activity Relationship
quat-C	Quaternary carbon
RCR	Risk characterization ratio
SpERC	Specific Environmental Release Category
STOT RE	Specific Target Organ Toxicity - Repeated Exposure
SVHC	Substance of Very High Concern
T	Toxic
U.S. EPA	United States Environmental Protection Agency
UVCB	Substances of Unknown or Variable composition, Complex reaction products or Biological materials
vPvB	very Persistent and very Bioaccumulative
WAF	Water accommodated fraction
WS	Water solubility
ww	wet weight