ECHA
EUROPEAN CHEMICALS AGENCY

Helsinki, 5 July 2019

Addressee: [redacted]

Decision number: CCH-D-2114465573-43-01/F
Substance name: Tris(2-ethylhexyl) phosphate
EC number: 201-116-6
CAS number: 78-42-2
Registration number: [redacted]
Submission number: [redacted]
Submission date: 27/03/2018
Registered tonnage band: Over 1000

DECISION ON A COMPLIANCE CHECK

Based on Article 41 of Regulation (EC) No 1907/2006 (the REACH Regulation), ECHA requests you to submit information on:

1. **Soil simulation testing (Annex IX, Section 9.2.1.3.; test method: Aerobic and anaerobic transformation in soil, EU C.23./OECD TG 307) at a temperature of 12 °C with the registered substance (i.e. the main constituent and relevant impurity present in concentrations at or above 0.1% (w/w) or, if not technically feasible, in concentrations as low as technically detectable);**

2. **Sediment simulation testing (Annex IX, Section 9.2.1.4.; test method: Aerobic and anaerobic transformation in aquatic sediment systems, EU C.24./OECD TG 308) at a temperature of 12 °C with the registered substance (i.e. the main constituent and relevant impurity present in concentrations at or above 0.1% (w/w) or, if not technically feasible, in concentrations as low as technically detectable);**

3. **Identification of degradation products (Annex IX, Section 9.2.3.) of the registered substance (i.e. the main constituent and relevant impurity present in concentrations at or above 0.1% (w/w) or, if not technically feasible, in concentrations as low as technically detectable);**

4. **Bioaccumulation in aquatic species (Annex IX, Section 9.3.2.; test method: Bioaccumulation in fish: aqueous and dietary exposure, OECD TG 305, dietary exposure) with the registered substance (i.e. the main constituent and relevant impurity present in concentrations at or above 0.1% (w/w) or, if not technically feasible, in concentrations as low as technically detectable);**

5. **Identification of PNEC and risk characterisation (Annex I, Section 3.3.1. and 6.): derive PNECs for freshwater, marine water, intermittent releases, freshwater sediment, marine sediment and soil**
   - using the study giving rise to the highest concern according to Annex I,

Section 3.1.5 and revise the risk characterisation accordingly *or* provide a detailed justification for not using the study giving rise to the highest concern;
- using the assessment factors recommended by ECHA and revise the risk characterisation accordingly *or* provide a detailed justification for not using.

You have to submit the requested information in an updated registration dossier by ***12 October 2022***. You shall also update the chemical safety report, where relevant.

The reasons of this decision are set out in Appendix 1. The procedural history is described in Appendix 2 and advice and further observations are provided in Appendix 3.

Appeal

This decision can be appealed to the Board of Appeal of ECHA within three months of its notification. An appeal, together with the grounds thereof, has to be submitted to ECHA in writing. An appeal has suspensive effect and is subject to a fee. Further details are described under: http://echa.europa.eu/regulations/appeals.

Authorised[1] by **Wim De Coen**, Head of Unit, Hazard Assessment.

[1] As this is an electronic document, it is not physically signed. This communication has been approved according to ECHA's internal decision-approval process.

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Appendix 1: Reasons

1. Soil simulation testing (Annex IX, Section 9.2.1.3.)

In accordance with Articles 10(a) and 12(1) of the REACH Regulation, a technical dossier registered at more than 1000 tonnes per year must contain, as a minimum, the information specified in Annexes VII to X to the REACH Regulation. The information to be generated for the dossier must fulfil the criteria in Article 13(4) of the same regulation.

"Soil simulation testing" is a standard information requirement as laid down in Annex IX, section 9.2.1.3. of the REACH Regulation for substances with a high potential for adsorption to soil. The registered substance has low water solubility (0.14 µg/L), high partition coefficient (log Kow ≥ 6.26) and high adsorption coefficient (log Koc: 6.3-6.4), indicating high adsorptive properties. Therefore, adequate information on this endpoint needs to be present in the technical dossier for the registered substance to meet this information requirement.

You have sought to adapt this information requirement according to Annex IX, Section 9.2., column 2. You provided the following justification for the adaptation:
"Annex VIII & IX of REACH, Section 9.2, Column 2 states that:

"Further biotic degradation testing shall be proposed by the registrant if the chemical safety assessment according to Annex I indicates the need to investigate further the degradation of the substance and its degradation products. The choice of the appropriate test(s) depends on the results of the chemical safety assessment and may include simulation testing in appropriate media (e.g. water, sediment or soil)."

ECHA Guidance (R.7b) offers confirmatory statements in support of this general column 2 adaptation: "This (column 2 wording) may be taken as providing a general framework by which the exclusion of certain testing may be justified by the need to clarify or revise the conclusions of the CSA." And "An exposure assessment can be carried out on the basis of information on ready biodegradability. If an environmental risk assessment of a substance leads to the conclusion no risk, using only information on ready biodegradability, then there is no need for further testing of the biodegradability. However, further testing of the biodegradability (and/or ecotoxicity) of the substance may be required, if the risk assessment indicates a potential risk to one or more environmental compartments."

The registrant proposes that the chemical safety assessment for this substance concludes that as a result of carrying out steps a to d under REACH Article 14(3), the substance does not meet the criteria for classification as dangerous according to Regulation (EC) 1272/2008. As such, no exposure estimation (PEC estimation) or risk characterisation is required. Additionally, the substance is concluded by the registrant as not being PBT or vPvB, as it does not meet the bioaccumulation or toxicity criteria.

Annex X of REACH also requires registrants to identify degradation products, unless the substance is readily biodegradable. Normally this endpoint is achieved through the conduct of a simulation study conducted in water, sediment or soil. This endpoint is designed to identify where, as a result of transformation processes in the environment, transformation products may have the potential to be hazardous (or PBT vPvB). To this end, the registrant has addressed the endpoint of identification of degradation products in a weight of evidence argument. Data from the phototransformation in water study suitably identified two major

degradation products of tris(2-ethylhexyl)phosphate, 2-ethylhexanol and 2-ethylhexanoic acid. The data permits the conclusion that the degradation pathway for this substance results in the parent molecule transforming to 2-ethylhexanol, which is then subsequently transformed to 2-ethylhexanoic acid. Both of these transformation products are considered non-hazardous to the environment and are not considered PBT or vPvB. In addition to this assessment of abiotic transformation, the Registrant assessed biologically mediated transformation of the chemical substance using the EAWAG-BBD Pathway Prediction System, which predicts pathways for microbial degradation of chemical compounds (see Section 5.6 of IUCLID). Predictions use biotransformation rules, based on reactions found in the EAWAG-BBD database or in the scientific literature. The BBD database contains information on microbial biocatalytic reactions and biodegradation pathways for primarily xenobiotic chemical compounds. The goal of the EAWAG-BBD is to provide information on microbial enzyme-catalyzed reactions that are important for biotechnology. The reactions covered are studied for basic understanding of nature, biocatalysis leading to specialty chemical manufacture, and biodegradation of environmental pollutants. Individual reactions and metabolic pathways are presented with information on the starting and intermediate chemical compounds, the organisms that transform the compounds, the enzymes, and the genes. The EAWAG-BBD Pathway Prediction System was consistent with the degradation processes observed in the phototransformation study, indicating that regardless of whether transformation of this substance is abiotically or biotically-mediated, the transformation of the parent molecule follows the same route, with the primary transformation product being 2-ethylhexanol and the secondary transformation product being 2-ethylhexanoic acid. As such, the degradation products for this substance are considered to be suitably identified in accordance with Annex X, Section 9.2.3 of thee REACH Regulation."

However, ECHA notes that your adaptation does not meet the specific rules for adaptation set by Column 2 of Annex IX, Sections 9.2 and 9.2.1.3.

Degradation testing may be omitted based on the results of the chemical safety assessment. However, in your adaptation you refer to the ECHA Guidance R7b where it states that "*exposure assessment can be carried out on the basis of information on ready biodegradability"* if the Environmental Risk Assessment (ERA) leads to the conclusion no risk, while you also argue that exposure estimation (PEC estimation) and risk characterisation have not been performed due to "*the substance not meeting the criteria for classification as dangerous according to Regulation (EC) 1272/2008"*. Thus, you have not provided an appropriate documentation (i.e. exposure assessment and risk assessment) to show that the Chemical Safety Report (CSR) would indicate that there is no need for simulation testing.

In addition, in your adaptation you mention that "*The substance is concluded by the registrant as not being PBT or vPvB, as it does not meet the bioaccumulation or toxicity criteria*." However, ECHA considers that your Chemical Safety Assessment (CSA) does not demonstrate the absence of concerns for potential PBT/vPvB properties of the registered substance, including the relevant impurity, and the degradation products. Only negligible biodegradation of the registered substance was observed in the ready biodegradability test, therefore it is potentially P and vP. The registered substance has a high potential for bioaccumulation (Kow >4.5) and the information provided to fulfil the bioaccumulation endpoint cannot be accepted (see section 3 Appendix 1 of the present draft decision). As for toxicity, information is currently incomplete in your registration dossier. Therefore, it is not possible to rule out that the registered substance could meet the T criteria. Consequently, ECHA considers that your CSA does indicate the need to investigate further the degradation

of the registered substance (including the impurity) and its degradation products for the assessment of its potential PBT/vPvB properties.

ECHA also notes that you provided information on degradation products in your justification for the adaptation of this information requirement, based on a weight of eveidnence. However, identification of the degradation products of the registered substance as explained, under Sect "3." below, is incomplete, because it does not consider a relevant impurity.

Acording to Annex IX, Section 9.2.1.3, column 2 of the REACH Regulation, simulation testing on soil does further not need to be conducted if the substance is readily biodegradable or if direct or indirect exposure of soil is unlikely. ECHA notes only negligible degradation of the registered substance was observed in the ready biodegradability tests presented in the registration dossier, OECD 301B (0.76% degradation in 28 days and 1.2% degradation in 56 days ([redacted] 2017), and 9.6% degradation in 28 days ([redacted] 2013)), OECD 301D (4% degradation in 28 days, 1% degradation in 56 days , [redacted] 2014), OECD 301C (0% degradation in 28 days, CITI 1992). Therefore, the registered substance is not readily biodegradable.

Finally, regarding exposure of soil, the registered substance has a low water solubility 0.14 µg/L, high partition coefficient (log Kow ≥ 6.26) and high adsorption coefficient (log Koc: 6.3-6.4) indicating adsorptive properties. Furthermore, based on the uses reported in the technical dossier, ECHA considers that soil exposure is expected (i.e. use in plant protection products [redacted] ERC 8d) and for other reported uses it cannot be excluded (e.g. Environmental Release Category (ERC) 4, 5,10a, 10b and 11a). Moreover, ECHA considers that soil exposure cannot be excluded as there are no exposure estimations in the Chemical Safety Report (CSR). ECHA therefore considers that you have not demonstrated that soil exposure is unlikely.

In view of the above, ECHA concludes that you have not demonstrated that the requirements of any of the specific rules for adaptation presented in column 2 of Annex IX, Section 9.2 of the REACH Regulation are met. Therefore, your adaptation of the information requirement cannot be accepted.

As explained above, the information provided on this endpoint for the registered substance in the technical dossier does not meet the information requirements. Consequently there is an information gap and it is necessary to provide information for this endpoint.

According to ECHA *Guidance on information requirements and chemical safety assessment, Chapter R.7b* (version 4.0, June 2017) Aerobic and anaerobic transformation in soil (test method EU C.23. / OECD TG 307) is the preferred test to cover the standard information requirement of Annex IX, Section 9.2.1.3.

One of the purposes of the simulation test is to provide the information that must be considered for assessing the P/vP properties of the registered substance in accordance with Annex XIII of REACH Regulation to decide whether it is persistent in the environment.

According to Annex XIII of REACH, the identification of PBT/vPvB substances shall take account of the PBT/vPvB-properties of relevant constituents of the substance. Impurities present in concentrations at or above 0.1 % (w/w) are deemed to be relevant constituents of the substance. Indeed, Section R.11.4.1 (page 33) of REACH Guidance document R.11 on PBT/vPvB assessment (version 2.0, November 2014) indicates that "*constituents, impurities*

and additives are relevant for the PBT/vPvB assessment when they are present in concentration of ≥ 0.1% (w/w). This limit of 0.1% (w/w) is set based on a well-established practice rooted in a principle recognised in European Union legislation". Therefore the biodegradation should be assessed for the main constituent and relevant impurity present in the registered substance in concentrations at or above 0.1% (w/w) or, if not technically feasible, in concentrations as low as technically detectable.

ECHA notes that the registered substance composition includes the impurity [redacted] which has been included in the inventory of substances likely to meet the criteria of Annex III to the REACH Regulation, due to e.g. its suspected persistency in the environment based on QSARs[2]. The impurity is reported in the technical dossier to be in concentrations between [redacted] (w/w), typical concentration [redacted] (w/w). Thus, it is above >0.1% (w/w).

Annex XIII also indicates that "*the information used for the purposes of assessment of the PBT/vPvB properties shall be based on data obtained under relevant conditions*". The Guidance on information requirements and chemical safety assessment R.7b (version 4.0, June 2017) specifies that simulation tests "attempt to simulate degradation in a specific environment by use of indigenous biomass, media, relevant solids [...], and a typical temperature that represents the particular environment". The Guidance on information requirements and chemical safety assessment Chapter R.16 on Environmental Exposure Estimation, Table R.16-8 (version 3.0 February 2016) indicates 12°C (285K) as the average environmental temperature for the EU to be used in the chemical safety assessment. Performing the test at the temperature of 12°C is within the applicable test conditions of the Test Guideline OECD TG 307. Therefore, the test should be performed at the temperature of 12°C.

Simulation tests performed in sediment or in soil possibly imply the formation of non-extractable residues (NER). These residues (of the parent substance and/or transformation products) are bound to the soil or to the sediment particles. NERs may potentially be re-mobilised as parent substance or transformation product unless they are irreversibly bound or incorporated into the biomass. When reporting the non-extractable residues (NER) in your test results you should explain and scientifically justify the extraction procedure and solvent used obtaining a quantitative measure of NER.

In your comments on the draft decision according to Article 50(1) of the REACH Regulation you agree on performing this simulation test on the radiolabelled tris(2-ethylhexyl)phosphate.

Besides, you propose a testing strategy for the impurity, where first an OECD 301 biodegradability testing would be performed following ECHA Guidance R.7. Following this study, you suggest to only perform the experimental OECD TG 307 in case that the pass level of OECD TG 301 is not reached, the process optimization of the manufacture does not decrease the impurity concentration to levels below 0.1%, and the calculated BCFmax > 2000 with Dimitrov model.

ECHA agrees with your testing strategy, except for using the calculated BCFmax ≤2000 with Dimitrov model as a condition not to perform the simulation test. Following ECHA *Guidance on information requirements and chemical safety assessment, Chapter R.11.4.1.2.* (version

[2] https://echa.europa.eu/information-on-chemicals/annex-iii-inventory/-/dislist/details/AIII-100.030.362

3.0, June 2017), QSARs can only be used in a Weight-of-Evidence approach for the B and vB assessment.

Therefore, pursuant to Article 41(1) and (3) of the REACH Regulation, you are requested to submit the following information derived with the registered substance subject to the present decision: Aerobic and anaerobic transformation in soil (test method: EU C.23./OECD TG 307). The biodegradation of the main constituent and relevant impurity present in concentration at or above 0.1% (w/w) or, if not technically feasible, in concentrations as low as technically detectable shall be assessed. This can be done simultaneously during the same study.

2. Sediment simulation testing (Annex IX, Section 9.2.1.4.)

In accordance with Articles 10(a) and 12(1) of the REACH Regulation, a technical dossier registered at more than 1000 tonnes per year must contain, as a minimum, the information specified in Annexes VII to X to the REACH Regulation. The information to be generated for the dossier must fulfil the criteria in Article 13(4) of the same regulation.

"Sediment simulation testing" is a standard information requirement as laid down in Annex IX, section 9.2.1.4. of the REACH Regulation for substances with a high potential for adsorption to sediment. The registered substance has low water solubility (0.14 µg/L), high partition coefficient (log Kow ≥ 6.26) and high adsorption coefficient (log Koc: 6.3-6.4), indicating high adsorptive properties. Therefore, adequate information on this endpoint needs to be present in the technical dossier for the registered substance to meet this information requirement.

You have sought to adapt this information requirement according to Annex IX, Section 9.2., column 2 by providing principally the same justification as for adaptation of the soil simulation testing above. However, as already explained in detail in section "2." above, the need to investigate further the degradation based on the chemical safety assessment cannot be excluded. The Substance cannot be considered readily biodegradable. Regarding exposure of sediment, the substance has a low water solubility 0.14 µg/L, high partition coefficient (log Kow ≥ 6.26) and high adsorption coefficient (log Koc: 6.3-6.4) indicating adsorptive properties. Furthermore, based on the uses reported in the technical dossier, ECHA considers that such uses are reported for which sediment exposure cannot be excluded (e.g. Environmental Release Category (ERC) 4, 5, 8d, 10a, 10b and 11a). Moreover, ECHA considers that sediment exposure cannot be excluded as there are no exposure estimations in the Chemical Safety Report (CSR). ECHA therefore considers that you have not demonstrated that sediment exposure is unlikely.

Therefore, your adaptation of the information requirement cannot be accepted.

As explained above, the information provided on this endpoint for the registered substance in the technical dossier does not meet the information requirements. Consequently there is an information gap and it is necessary to provide information for this endpoint.

According to ECHA *Guidance on information requirements and chemical safety assessment, Chapter R.7b* (version 4.0, June 2017) Aerobic and anaerobic transformation in aquatic sediment systems (test method EU C.24. / OECD TG 308) is the preferred test to cover the standard information requirement of Annex IX, Section 9.2.1.4.

One of the purposes of the simulation test is to provide the information that must be considered for assessing the P/vP properties of the registered substance in accordance with Annex XIII of REACH Regulation to decide whether it is persistent in the environment.

According to Annex XIII of REACH, the identification of PBT/vPvB substances shall take account of the PBT/vPvB-properties of relevant constituents of the substance. Impurities present in concentrations at or above 0.1 % (w/w) are deemed to be relevant constituents of the substance. Indeed, Section R.11.4.1 (page 33) of REACH Guidance document R.11 on PBT/vPvB assessment (version 2.0, November 2014) indicates that "*constituents, impurities and additives are relevant for the PBT/vPvB assessment when they are present in concentration of ≥ 0.1% (w/w). This limit of 0.1% (w/w) is set based on a well-established practice rooted in a principle recognised in European Union legislation*". Therefore the biodegradation should be assessed for main constituent and relevant impurity present in the registered substance in concentrations at or above 0.1% (w/w) or, if not technically feasible, in concentrations as low as technically detectable.

ECHA notes that notes that the registered substance composition includes the impurity, [redacted] which has been included in Annex III inventory due to being suspected e.g. persistency in the environment based on QSARs[3]. The impurity is reported in the technical dossier to be in concentrations between [redacted] (w/w), typical concentration [redacted] (w/w). Thus, it is above >0.1% (w/w).

Annex XIII also indicates that "*the information used for the purposes of assessment of the PBT/vPvB properties shall be based on data obtained under relevant conditions*". The Guidance on information requirements and chemical safety assessment R.7b (version 4.0, June 2017) specifies that simulation tests "attempt to simulate degradation in a specific environment by use of indigenous biomass, media, relevant solids [...], and a typical temperature that represents the particular environment". The Guidance on information requirements and chemical safety assessment Chapter R.16 on Environmental Exposure Estimation, Table R.16-8 (version 3.0 February 2016) indicates 12°C (285K) as the average environmental temperature for the EU to be used in the chemical safety assessment. Performing the test at the temperature of 12°C is within the applicable test conditions of the Test Guideline OECD TG 308. Therefore, the test should be performed at the temperature of 12°C.

Simulation tests performed in sediment or in soil possibly imply the formation of non-extractable residues (NER). These residues (of the parent substance and/or transformation products) are bound to the soil or to the sediment particles. NERs may potentially be re-mobilised as parent substance or transformation product unless they are irreversibly bound or incorporated into the biomass. When reporting the non-extractable residues (NER) in your test results you should explain and scientifically justify the extraction procedure and solvent used obtaining a quantitative measure of NER.

In your comments on the draft decision according to Article 50(1) of the REACH Regulation you agree on performing this simulation test on the radiolabelled tris(2-ethylhexyl)phosphate.

Besides, you propose a testing strategy for the impurity, where first an OECD 301 biodegradability testing would be performed following ECHA Guidance R.7. Following this study, you suggest to only perform the experimental OECD TG 308 in case that the pass

[3] https://echa.europa.eu/information-on-chemicals/annex-iii-inventory/-/dislist/details/AIII-100.030.362

level of OECD TG 301 is not reached, the process optimization of the manufacture does not decrease the impurity concentration to levels below 0.1%, and the calculated BCFmax > 2000 with Dimitrov model.

ECHA agrees with your testing strategy, except for using the calculated BCFmax ≤2000 with Dimitrov model as a condition not to perform the simulation test. Following ECHA *Guidance on information requirements and chemical safety assessment, Chapter R.11.4.1.2.* (version 3.0, June 2017), QSARs can only be used in a Weight-of-Evidence approach for the B and vB assessment.

Therefore, pursuant to Article 41(1) and (3) of the REACH Regulation, you are requested to submit the following information derived with the registered substance subject to the present decision: Aerobic and anaerobic transformation in aquatic sediment systems (test method: EU C.24./OECD TG 308). The biodegradation of the main constituent and relevant impurity present in concentration at or above 0.1% (w/w) or, if not technically feasible, in concentrations as low as technically detectable shall be assessed. This can be done simultaneously during the same study.

Notes for your consideration for Sections 1 and 2

Before conducting the requested tests you are advised to consult the ECHA Guidance on information requirements and chemical safety assessment, Chapter R7b, Sections R.7.9.4 and R.7.9.6 (version 4.0, June 2017) and Chapter R.11, Section R.11.4.1.1 (version 3.0, June 2017) on PBT assessment to determine the sequence in which the simulation tests are to be conducted and the necessity to conduct all of them. The order in which the simulation biodegradation tests are performed needs to take into account the intrinsic properties of the registered substance and the identified use and release patterns which could significantly influence the environmental fate of the registered substance .

In accordance with Annex I, Section 4, of the REACH Regulation you should revise the PBT assessment when results of the tests detailed above is available. You are also advised to consult the ECHA Guidance on information requirements and chemical safety assessment (version 3.0, June 2017), Chapter R.11, Section R.11.4.1.1. and Figure R. 11-3 on PBT assessment for the integrated testing strategy for persistency assessment in particular taking into account the degradation products of the registered substance.

3. Identification of degradation products (Annex IX, Section 9.2.3.)

The identification of the degradation products is a standard information requirement according to column 1, Section 9.2.3. of Annex IX of the REACH Regulation. Adequate information on this endpoint needs to be present in the technical dossier for the registered substance to meet this information requirement.

The biodegradation section in the technical dossier does not contain any information in relation to the identification of degradation products, nor an adaptation in accordance with column 2 of Annex IX, Sections 9.2 or 9.2.3. or with the general rules of Annex XI for this standard information requirement. "

In the technical dossier you have provided information on degradation products in a weight of evidence argument. Data on abiotic degradation products from a phototransformation in water study (OECD TG 316, 2013) performed with the registered substance has been provided. Besides, a prediction perfomed with EAWAG-BBD Pathway Prediction System on

the main constituent of the registered substance, Tris(2 -ethylhexyl) phosphate, has been provided. However, this information does not provide the information required by Annex IX, Section 9.2.3., because it does not include the biotic and abiotic degradation products of the whole registered substance, which includes the relevant impurity, [redacted]

According to Annex XIII of REACH, the identification of PBT/vPvB substances shall take account of the PBT/vPvB-properties of relevant constituents of the substance. Impurities present in concentrations at or above 0.1 % (w/w) are deemed to be relevant constituents of the substance. Indeed, Section R.11.4.1 (page 33) of REACH Guidance document R.11 on PBT/vPvB assessment (version 2.0, November 2014) indicates that "*constituents, impurities and additives are relevant for the PBT/vPvB assessment when they are present in concentration of ≥ 0.1% (w/w). This limit of 0.1% (w/w) is set based on a well-established practice rooted in a principle recognised in European Union legislation*". Therefore the degradation products should be assessed for main constituent and relevant impurity present in the registered substance in concentrations at or above 0.1% (w/w) or, if not technically feasible, in concentrations as low as technically detectable.

ECHA notes that the registered substance composition includes the [redacted] which has been included in Annex III inventory due to being suspected e.g. persistency in the environment based on QSARs[4]. The impurity is reported in the technical dossier to be in concentrations between [redacted] (w/w), typical concentration [redacted] (w/w). Thus, it is above >0.1% (w/w).

ECHA considers that this information is needed in relation to the PBT/vPvB assessment and risk assessment.

As explained above, the information provided on this endpoint for the registered substance in the technical dossier does not meet the information requirements. Consequently there is an information gap and it is necessary to provide information for this endpoint.

Regarding appropriate and suitable test method, the methods will have to be substance-specific. When analytically possible, identification, stability, behaviour, molar quantity of metabolites relative to the parent compound should be evaluated. In addition, degradation half-life, log Kow and potential toxicity of the metabolite may be investigated. You may obtain this information from the simulation studies also requested in this decision (Sections 1 and 2, above), or by some other measure. You will need to provide a scientifically valid justification for the chosen method.

In your comments on the draft decision according to Article 50(1) of the REACH Regulation you request clarification on how information on log Kow and potential toxicity of a metabolite may be obtained from the abovementioned simulation tests.

ECHA acknolwedges your need for clarification. Simulation tests per se cannot provide with information on the log Kow and potential toxicity of the metabolites. Nevertheless, the identification of the metabolites through the simulation tests, allow further assessment of these.

[4] https://echa.europa.eu/information-on-chemicals/annex-iii-inventory/-/dislist/details/AIII-100.030.362

Therefore, pursuant to Article 41(1) and (3) of the REACH Regulation, you are requested to submit the following information derived with the registered substance subject to the present decision:

Identification of the degradation products (Annex IX, Section 9.2.3.) of the main constituent and relevant impurity present in concentration at or above 0.1% (w/w) or, if not technically feasible, in concentrations as low as technically detectable shall be assessed, by using an appropriate and suitable test method, as explained above in this section.

3. Bioaccumulation in aquatic species (Annex IX, Section 9.3.2.)

In accordance with Articles 10(a) and 12(1) of the REACH Regulation, a technical dossier registered at more than 1000 tonnes per year must contain, as a minimum, the information specified in Annexes VII to X to the REACH Regulation. The information to be generated for the dossier must fulfil the criteria in Article 13(4) of the same regulation.

"Bioaccumulation in aquatic species, preferably fish" is a standard information requirement as laid down in Annex IX, Section 9.3.2.of the REACH Regulation. Adequate information on this endpoint needs to be present in the technical dossier for the registered substance to meet this information requirement.

In the technical dossier you have provided study records for an experimental result with common carp ([redacted], 1985), for a QSAR prediction performed with the model BCFBAF v4.11 (a module of the EPISuite program), and for a QSAR prediction with the model Dimitrov 2005 (manually calculated according to publication[5]). From the experimental study, a BCF of 22 was reported. From the BCFBAF QSAR model, a bioconcentration factor (BCF) of 30.34 was predicted. From the Dimitrov QSAR model, a bioconcentration factor (BCF) of 336.6 was predicted. For your chemical safety assessment (CSA) you have assumed a BCF value of 22, i.e., the result from the experimental study.

Your dossier reports data from a an experimental result with a test guideline equivalent or similar to OECD TG 305C ([redacted], 1985), where *Cyprinus carpio* was exposed through water to the registered substance. The registered substance was dosed into the system to achieve 2 and 0.2 mg/L, for which acetone was used as solvent (the use of 200 and 20 mg/L acetone was reported).

ECHA notes that the aqueous exposure concentration exceeded the water solubility of the registered substance (i.e. 0.14 µg/L). Moreover, the used solvent concentration exceeded the acceptable amount of 100 mg/L, as you already reported in the technical dossier.

In addition, some other quality concerns in the reported study are:

- The study only consisted of an uptake phase with no depuration phase as significant uptake was not achieved after 42 days.
- Due to the availability of data it is not possible to determine a BCFss or BCFk from the study.

[5] S. Dimitrov, N. Dimitrova, T. Parkerton, M. Comber, M. Bonnell & O. Mekenyan (2005) Base-line model for identifying the bioaccumulation potential of chemicals, SAR and QSAR in Environmental Research, 16:6, 531-554, DOI: 10.1080/10659360500474623

- Acetone was used but at varying amounts for the two concentrations, acetone addition when used as a solvent should remain the same in all exposures.
- It is unclear if a solvent control was tested alongside the exposures to TEHP and the water only control.
- The time of sampling is also important and it is unclear when this occured. Sampling should occur before feeding, water samples should also be taken before the addition of fish; details on these are lacking.
- Whether fish mortality occured during exposure was not reported.

Given the abovementioned reasons, and as you state in the overall remark of the robust study summary, "*from the report many important annexes are missing which contain raw data, however the study would still remain deficient*", ECHA concludes that the BCF you have used for the assessment of bioaccumulation is uncertain, since the reliability of the provided experimental results cannot be guaranteed. Therefore, the results from this study do not provide the information required by Annex IX, Section 9.3.2., and are not adequate to conclude on the bioaccumulation potential of the registered substance

The QSAR models you have used for your assessment predicts a log BCF value from log Kow for the main constituent of the registered substance. EPISUIT BCFBAF is based on 3 distinct linear regression equations, depending on whether Log Kow is < 1.0, between 1.0 and 7.0, or > 7.0. ECHA notes that you have used a log Kow value estimated from KOWWIN, that is 9.49, as input to the model. However, it is apparent in the documentation of the BCFBAF v4.11 model that the goodness of fit for chemicals with log Kow > 7 is very poor. Therefore, the model's predictions for substance with very high log Kow are regarded as uncertain.

ECHA notes that for the predicton of Dimitrov et al. (2005), you have used e the KOWWIN estimated logKow (9.49). ECHA notes that the estimated value is yet not a certain value, and that the modelling of an uncertain value would provide an uncertain prediction.

ECHA concludes, that the reliability of both QSAR predictions you have used for the bioaccumulation endpoint are uncertain for the reasons mentioned above.

Moreover, both QSAR predictions attempted to predict the BCF for the main constituent of the registered substance, only. ECHA notes that no complementary specific information on the impurity [redacted] has been included in the registration dossier, which has been included in Annex III inventory due to suspected e.g. persistency in the environment based on QSARs[6]. The impurity is reported in the technical dossier to be in concentrations between [redacted] (w/w), typical concentration [redacted] (w/w). Thus, it is above >0.1% (w/w).

It should also be noted that according to Annex XIII of REACH, the identification of PBT/vPvB substances shall take account of the PBT/vPvB-properties of relevant constituents of the substance. Impurities present in concentrations at or above 0.1 % (w/w) are deemed to be relevant constituents of the substance. Indeed, Section R.11.4.1 (page 33) of REACH Guidance document R.11 on PBT/vPvB assessment (version 2.0, November 2014) indicates that "*constituents, impurities and additives are relevant for the PBT/vPvB assessment when they are present in concentration of ≥ 0.1% (w/w). This limit of 0.1% (w/w) is set based on a well-established practice rooted in a principle recognised in European Union legislation*". Moreover, REACH Guidance document R.11 on PBT/vPvB assessment (version 2.0,

[6] https://echa.europa.eu/information-on-chemicals/annex-iii-inventory/-/dislist/details/AIII-100.030.362

November 2014) Section R.11.3.2.1., also states that for the PBT/vPvB assessment, the bioaccumulation or bioconcentration potential of degradation products shall also be investigated.

Therefore, the WoE of the QSAR predictions and the experimental study do not provide the information required by Annex IX, Section 9.3.2., and are not adequate to conclude on the bioaccumulation potential of the registered substance.

Therefore, your adaptation of the information requirement cannot be accepted.

As explained above, the information provided on this endpoint for the registered substance in the technical dossier does not meet the information requirement. Consequently there is an information gap and it is necessary to provide information for this endpoint.

According to *ECHA Guidance on information requirements and chemical safety assessment, Chapter R.7c* (version 3.0, June 2017) bioaccumulation in fish: aqueous and dietary exposure (test method EU C.13. / OECD TG 305) is the preferred test to cover the standard information requirement of Annex IX, Section 9.3.2. of the REACH Regulation.

ECHA Guidance defines further that results obtained from a test with aqueous exposure can be used directly for comparison with the B and vB criteria of Annex XIII of REACH Regulation and can be used for hazard classification and risk assessment. Comparing the results of a dietary study with the REACH Annex XIII B and vB criteria is more complex and has higher uncertainty. Therefore, the aqueous route of exposure is the preferred route and shall be used whenever technically feasible. If you decided to conduct the study using the dietary exposure route, you shall provide scientifically valid justification for your decision. You shall also attempt to estimate the corresponding BCF value from the dietary test data by using the approaches given in Annex 8 of the OECD 305 TG and in OECD Guidance Document on Aspects of OECD TG 305 on Fish Bioaccumulation, ENV/JM/MONO (2017)16. In any case you shall report all data derived from the dietary test as listed in the OECD 305 TG.

In your comments on the draft decision according to Article 50(1) of the REACH Regulation you propose a testing strategy, for the main constituent and for the impurity. You suggest to conduct a new OECD TG 123 study on the main constituent and on the impurity, in a laboratory with a sufficiently sensitive analytical method in order to apply Dimitrov model with a discrete experimental Log Kow value. Following to this, in the case of tris(2-ethylhexyl) phosphate, you propose to perform the dietary OECD TG 305, if the calculated BCFmax >2000 with Dimitrov model and if it is concluded P. In the case of the impurity, you propose to perform the OECD TG 305, if a non-successful process optimization of the manufacture, the calculated BCFmax >2000 with Dimitrov model and it is concluded P.

ECHA agrees with your testing strategy proposal, except for using the calculated BCFmax ≤2000 with Dimitrov model as a condition not to perform the dietary OECD 305 TG. As mentioned above (Sections 1 and 2 in the present decision), following ECHA *Guidance on information requirements and chemical safety assessment, Chapter R.11.4.1.2* (version 3.0, June 2017), QSARs can only be used in a Weight of-Evidence approach for the B and vB assessment. Furthermore:

Available screening information indicates potential B properties for the main constituent.

Annex XIII of the REACH Regulation makes the distinction between 'screening information' and 'assessment information'.

Section 2.1. of this Annex specifies that "*no additional information needs to be generated for the assessment of PBT/vPvB properties if there is no indication of P or B properties following the result from the screening test or other information*". Therefore, as long as one piece of screening information indicates that the substance could potentially be bioaccumulative (B) or very bioaccumulative (vB), then further information will need to be generated.

Section 3.1.2. of Annex XIII of the REACH Regulation indicates that the log Kow of the substance can constitute screening information for the assessment of B and vB properties. Chapter R.11 of the ECHA *Guidance on information requirements and chemical safety assessment* (version 3.0, June 2017), specifies that the threshold value for screening for B and vB properties is log Kow greater than 4.5.

ECHA notes that you have reported for the main constituent an experimental log Kow value which is above 6.26, although ECHA understands that the actual log Kow may be higher. Therefore, ECHA concludes that the screening criterion of log Kow >4.5 is positively met for the main constituent. Consequently, there is indication of B properties from the available screening information for the main constituent.

Regarding the impurity, ECHA notes that in your comments you mention that no experimentally determined log KOW value is available for [redacted] although for the structurally close analogue [redacted] a log Kow> 5.7 was experimentally determined. If this read-across would be valid, there would also be indication of potential B properties of the impurity.

A QSAR prediction cannot be regarded as assessment information

Section 3.2. of Annex XIII of the REACH Regulation presents 'assessment information' that could be used to conclude on the PBT/vPvB status of a substance. However, ECHA notes that QSAR predictions are not mentioned as possible assessment information. Therefore, ECHA considers that the BCF value predicted by Dimitrov model cannot be regarded as assessment information that would supersede the screening information represented by the log Kow of >6.26.

ECHA further ackowledges your comment that the information on the used LogKow for the Dimitrov model derivation was present in the technical dossier and overlooked by ECHA. ECHA has revised the relevant text in this request, accordingly.

Therefore, pursuant to Article 41(1) and (3) of the REACH Regulation, you are requested to submit the following information derived with the registered substance subject to the present decision: Bioaccumulation in fish: aqueous or dietary bioaccumulation fish test (test method: OECD TG 305). The bioaccumulation of the main constituent and relevant impurity present in concentration at or above 0.1% (w/w) or, if not technically feasible, in concentrations as low as technically detectable shall be assessed. This can be done

simultaneously during the same study. For the PBT/vPvB assessment, the bioaccumulation or bioconcentration potential of degradation products shall also be investigated.

Note for your consideration

Before conducting the above test you are advised to consult the ECHA *Guidance on information requirements and chemical safety assessment* (version 3.0, June 2017), Chapter R.11.4. and Figure R.11-4 on the PBT assessment for further information on the integrated testing strategy for the bioaccumulation assessment of the registered substance. In particular, you are advised to first conclude whether the registered substance may fulfil the REACH Annex XIII criteria of being persistent or very persistent, and then to consult the PBT assessment for Weight-of-Evidence determination and integrated testing strategy for bioaccumulation assessment. You should revise the PBT assessment when information on bioaccumulation is available.

4. Identification of PNEC and risk characterisation (Annex I, Sections 3.3.1. and 6.)

In accordance with Articles 10(b) and 14(1) of the REACH Regulation, the registration must contain a chemical safety report (CSR) which documents the chemical safety assessment (CSA) conducted in accordance with Article 14(2) to (7) and with Annex I to the REACH Regulation.

Annex I, Section 3.3.1. of the REACH Regulation requires to establish a predicted no effect concentration (PNEC) for each environmental sphere based on the available information and to use an appropriate assessment factor to the effect values.

The ECHA *Guidance on information requirements and chemical safety assessment,* Chapter R.10 (May 2008), provides further details and specifically provides default factors which should be applied to derive PNECs.

Further, according to Annex I, Section 3.3.2., if it is not possible to derive the PNEC, then this shall be clearly stated and fully justified.

You have not established the PNECs for freshwater, marine water and intermittent releases using the following justification: "*... In accordance with tiered testing requirements under REACH Annexes VII to X, no short-term or long-term adverse effects were observed in aquatic organisms when tested up to, and over, the limit of solubility of the substance. Refer to IUCLID Section 6.1. for detailed information. "*

ECHA notes that, PNEC freshwater can be calculated using assessment factors also for substances that do not show toxicity in short-term tests, if the log Kow > 3 (or BCF > 100) and if the PEClocal/regional is > 1/100th of the water solubility. In such cases, "*A long-term test has to be carried out (...). The long-term toxicity test should normally be a test on invertebrate (preferred species Daphnia) to avoid unnecessary vertebrate testing. The NOEC from this test can then be used with an assessment factor of 100. If in addition to the required long-term test a NOEC is determined from an algal test of the base-set, an assessment factor of 50 is applied.*"(ECHA *Guidance on information requirements and chemical safety assessment* (May 2008), Chapter R10, Section R10.3.1.2).

On the other hand, you have not established the PNECs for soil. You indicatethe following justification: "*no hazard identified*" and "t*esting on soil toxicity does not appear scientifically necessary. The already available studies on aquatic organisms indicate that neither in acute tests in 3 trophic levels nor in chronic tests in daphnia and algae any effects have been observed up to the limit of the water solubility of 0.14 µg/L*".

ECHA notes, you have not established PNEC sediment. You indicate that you have proposed a sediment-water Chironomid toxicity test to derive PNECsediment.
ECHA notes that currently there are two decisions (one adopted decision compliance check~~)~~ and a draft decision testing proposal) on this registered substance, where toxicity tests on soil and sediment organisms, respectively have been requested.

Therefore, derivation of PNECsoil and PNECsediment should be performed once the results of these tests are available, should they include these studies as part of the adopted decisions, using the study giving rise to the highest concern according to Annex I, Section 3.1.5, or providing a detailed justification for not using the study giving rise to the highest concern; and using the assessment factors in accordance with ECHA *Guidance on information requirements and chemical safety assessment,* Chapter R.10. (May 2008), or providing a detailed justification for not using these.

As explained above, the information provided on PNEC for the registered substance in the chemical safety report does not meet the general requirements for preparing a chemical safety report as described in Annex I, Section 3.3.1.. Consequently, it is necessary to derive the PNECs.

Therefore, pursuant to Article 41(1) and (3) of the REACH Regulation, you are requested to derive PNECs for freshwater, marine water, intermittent releases, freshwater sediment, marine sediment and soil:
- using the study giving rise to the highest concern according to Annex I, Section 3.1.5 and revise the risk characterisation accordingly *or* provide a detailed justification for not using the study giving rise to the highest concern;
- using the default assessment factors and other recommendations of ECHA Guidance R.10 and revise the risk characterisation accordingly *or* provide a detailed justification on how the chosen approach meets the general requirements for identification of the PNEC as described in Section 3.3. of Annex I if not using the recommendations of ECHA Guidance R.10 for PNEC derivation.

Deadline to submit the requested information in this decision

In the draft decision communicated to you the time indicated to provide the requested information was 39 months from the date of adoption of the decision. In your comments on the draft decision, you requested an extension of the timeline in order to optimise the manufacturing process remove the impurity [redacted] to levels below 0.1%. You did not indicate an exact amount of additional time needed, although you mentioned that *"less than 12 months do not appear realistic to optimize the respective continuous reaction and purification process including upscaling"*.

ECHA acknowledges your intended strategy. Nevertheless, ECHA notes that 39 months have been granted for the requests in the draft decision, only not to optimise the manufacturing process to remove the impurity. Therefore, ECHA has not modified the deadline of the decision.

Appendix 2: Procedural history

For the purpose of the decision-making, this decision does not take into account any updates of your registration after the date when the draft decision was notified to you under Article 50(1) of the REACH Regulation.

The compliance check was initiated on 30 November 2017.

The decision making followed the procedure of Articles 50 and 51 of the REACH Regulation, as described below:

ECHA notified you of the draft decision and invited you to provide comments.

ECHA took into account your comments and did not amend a request, and did not amend the deadline.

ECHA notified the draft decision to the competent authorities of the Member States for proposals for amendment.

As no amendments were proposed, ECHA took the decision according to Article 51(3) of the REACH Regulation.

Appendix 3: Further information, observations and technical guidance

1. This compliance check decision does not prevent ECHA from initiating further compliance checks on the present registration at a later stage.

2. Failure to comply with the requests in this decision, or to otherwise fulfil the information requirements with a valid and documented adaptation, will result in a notification to the enforcement authorities of your Member State.

3. In relation to the information required by the present decision, the sample of the substance used for the new tests must be suitable for use by all the joint registrants. Hence, the sample should have a composition that is suitable to fulfil the information requirement for the range of substance compositions manufactured or imported by the joint registrants.

   It is the responsibility of all joint registrants who manufacture or import the same substance to agree on the appropriate composition of the test material and to document the necessary information on their substance composition. In addition, it is important to ensure that the particular sample of the substance tested in the new tests is appropriate to assess the properties of the registered substance, taking into account any variation in the composition of the technical grade of the substance as actually manufactured or imported by each registrant.

   If the registration of the substance by any registrant covers different grades, the sample used for the new tests must be suitable to assess these grades. Finally there must be adequate information on substance identity for the sample tested and the grades registered to enable the relevance of the tests to be assessed.