Helsinki, 02 June 2021

Addressees
Registrants of CEM JS 7299-99-2 listed in the last Appendix of this decision

Date of submission of the dossier subject of this decision
17/05/2017

Registered substance subject to this decision, 'the Substance'
Substance name: 2,2-bis[[(2-ethyl-1-oxohexyl)oxy]methyl]propane-1,3-diyl bis(2-ethylhexanoate)
EC number: 230-743-8
CAS number: 7299-99-2

Decision number: Please refer to the REACH-IT message which delivered this communication (in format CCH-D-XXXXXXXXXX-XX-XX/F)

DECISION ON A COMPLIANCE CHECK

Under Article 41 of Regulation (EC) No 1907/2006 (REACH), you must submit the the information listed below by the deadline of ***8 March 2024***.

A. Information required from all the Registrants subject to Annex VII of REACH

1. Long-term toxicity testing on aquatic invertebrates (triggered by Annex VII, Section 9.1.1., column 2), also requested at C.2. below;

2. Growth inhibition study aquatic plants (Annex VII, Section 9.1.2.; test method EU C.3./OECD TG 201) ;

B. Information required from all the Registrants subject to Annex VIII of REACH

1. Long-term toxicity testing on fish (triggered by Annex VIII, Section 9.1.3., column 2), also requested at C.3. below;

2. Soil simulation testing (triggered by Annex VIII, Section 9.2., column 2), also requested at C.4. below;

3. Sediment simulation testing (triggered by Annex VIII, Section 9.2., column 2), with the Substance, also requested at C.5. below;

4. The identification of degradation products (triggered by Annex VIII, Section 9.2., column 2) also requested at C.6. below;

5. Bioaccumulation in aquatic species (triggered by Annex I, sections 0.6.1. and 4. in conjunction with Annex XIII, Section 2.1.), also requested at C.7. below.

C. Information required from all the Registrants subject to Annex IX of REACH

1. Long-term toxicity testing on aquatic invertebrates (Annex IX, Section 9.1.5.; test method EU C.20./OECD TG 211) ;

2. Long-term toxicity testing on fish (Annex IX, Section 9.1.6.; test method OECD TG 210) ;

3. Soil simulation testing (Annex IX, Section 9.2.1.3.; test method EU C.23./OECD TG 307) at a temperature of 12 °C;

4. Sediment simulation testing (Annex IX, Section 9.2.1.4.; test method EU C.24./OECD TG 308) at a temperature of 12 °C;

5. Identification of degradation products (Annex IX, 9.2.3.) using an appropriate test method among those requested above (4 -5)

6. Bioaccumulation in aquatic species (Annex IX, Section 9.3.2.; test method: Bioaccumulation in fish: aqueous and dietary exposure, OECD TG 305, dietary exposure;

The reasons for the request(s) are explained in the following appendices:

- Appendices entitled "Reasons to request information required under Annexes VII to IX of REACH", respectively.

Information required depends on your tonnage band

You must provide the information listed above for all REACH Annexes applicable to you, and in accordance with Articles 10(a) and 12(1) of REACH:

- the information specified in Annex VII to REACH, for registration at 1-10 tonnes per year (tpa), or as a transported isolated intermediate in quantity above 1000 tpa;
- the information specified in Annexes VII and VIII to REACH, for registration at 10-100 tpa;
- the information specified in Annexes VII, VIII and IX to REACH, for registration at 100-1000 tpa;

You are only required to share the costs of information that you must submit to fulfil your information requirements.

For certain endpoints, ECHA requests the same study from registrants at different tonnages. In such cases, only the reasoning why the information is required at lower tonnages is provided in the corresponding Appendices.

For the tonnage where the study is a standard information requirement, the full reasoning for the request including study design is given. Only one study is to be conducted; the registrants concerned must make every effort to reach an agreement as to who is to carry out the study on behalf of the other registrants under Article 53 of REACH.

How to comply with your information requirements

To comply with your information requirements you must submit the information requested by this decision in an updated registration dossier by the deadline indicated above. You must also update the chemical safety report, where relevant, including any changes to classification and labelling, based on the newly generated information.

You must follow the general testing and reporting requirements provided under the Appendix entitled "Requirements to fulfil when conducting and reporting new tests for REACH

purposes". In addition, you should follow the general recommendations provided under the Appendix entitled "General recommendations when conducting and reporting new tests for REACH purposes". For references used in this decision, please consult the Appendix entitled "List of references".

The studies relating to biodegradation and bioaccumulation are necessary for the PBT assessment (requests B.2 to B.4 and C.3 to C.6). However, to determine the testing needed to reach the conclusion on the persistency and bioaccumulation of the Substance you should consider the sequence in which these tests are performed and other conditions described in Appendix entitled "Requirements to fulfil when conducting and reporting new tests for REACH purposes".

Appeal
This decision, when adopted under Article 51 of REACH, may be appealed to the Board of Appeal of ECHA within three months of its notification to you. Please refer to http://echa.europa.eu/regulations/appeals for further information.

Failure to comply
If you do not comply with the information required by this decision by the deadline indicated above, ECHA will notify the enforcement authorities of your Member State.

Authorised[1] under the authority of Christel Schilliger-Musset, Director of 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.

Appendix A: Reasons to request information required under Annex VII of REACH

1. The long-term toxicity testing on aquatic invertebrates also requested at C.1. below (triggered by Annex VII, Section 9.1.1., column 2)

Short-term toxicity testing on aquatic invertebrates is an information requirement under Annex VII to REACH (Section 9.1.1.). Long-term toxicity testing on aquatic invertebrates must be considered (Section 9.1.1., Column 2) if the substance is poorly water soluble.

The Substance is poorly water soluble (<0.4 µg/L). Therefore, long-term toxicity testing is needed to accurately define the hazard of the Substance.

The examination of the information provided, as well as the selection of the requested test and the test design are addressed in Appendix C, section 1.

ECHA has adressed your comments to the draft decision in section C.1 below.

2. Growth inhibition study aquatic plants (Annex VII, Section 9.1.2.)

Growth inhibition study aquatic plants is a standard information requirement in Annex VII to REACH.

You have adapted this information requirement by using a Grouping of substances and read-across approach under Annex XI, Section 1.5.

You have provided a read-across justification document in the CSR.

You predict the properties of the Substance from the structurally similar substance: [redacted] (CAS No. [redacted] i.e. the source substance).

The source study that you have used in your read-across approach, Toxicity to aquatic algae and cyanobacteria, [redacted], 2003, corresponds to an Algae Growth Inhibition test performed according to the OECD TG 201.

You have provided the following reasoning for the prediction of toxicological properties:
"Based on structural similarities, as all members of this category of esters have a hydrophobic nature. Included tabulated data demonstrates similar characteristics across the group in terms of physico-chemical and toxicological behaviour".

ECHA understands that you predict the properties of the Substance using a read-across hypothesis which assumes that different compounds have the same type of effects. The properties of your Substance are predicted to be quantitatively equal to those of the source substance.

Annex XI, Section 1.5. specifies two conditions which must be fulfilled whenever a read-across approach is used. Firstly, there needs to be structural similarity between substances which results in a likelihood that the substances have similar physicochemical, toxicological and ecotoxicological properties so that the substances may be considered as a group or category. Secondly, it is required that the relevant properties of a substance within the group may be predicted from data for reference substance(s) within the group (read-across approach).

Additional information on what is necessary when justifying a read-across approach can be found in the ECHA Guidance R.6 and related documents.

ECHA notes the following shortcomings with regards to the predictions of (eco)toxicological properties.

A read-across hypothesis needs to be provided, establishing why a prediction for a toxicological or ecotoxicological property is reliable. This hypothesis should be based on recognition of the structural similarities and differences between the source substance(s) and your Substance[2]. It should explain why the differences in the chemical structures should not influence the toxicological/ ecotoxicological properties or should do so in a regular pattern.

Your read-across hypothesis is that the similarity in chemical structure and in some of the physicochemical and toxicological properties between the source substance(s) and your Substance is a sufficient basis for predicting the properties of your Substance for other endpoints.

Similarity in chemical structure and similarity of some of the physicochemical and toxicological properties does not necessarily lead to predictable or similar ecotoxicological properties in other endpoints. As described above, a well-founded hypothesis is needed to establish a reliable prediction for a ecotoxicological property, based on recognition of the structural similarities and differences between the source substance(s) and your Substance.

In your comments to the draft decision you stated that further information is available, providing a link to a GLP study performed according to OECD TG 201 (Alga, Growth Inhibition Test). Due to the limited information provided in this link, ECHA cannot make an independent assessment of the study (e.g. validity criteria, analytical monitoring, solvent concentration used, preparation of the concentrations tested). In addition, you indicate that you will update your dossier. Please note that this decision does not take into account updates of the registration dossiers after the date on which you were notified of the draft decision according to Article 50(1) of REACH (see section 5.4. of ECHA's Practical Guide "How to act in Dossier Evaluation").

Therefore, the information requirement is not fulfilled.

[2] *Guidance on information requirements and chemical safety assessment*, Chapter R.6: QSARs and grouping of chemicals.

Appendix B: Reasons to request information required under Annex VIII of REACH

1. The long term toxicity testing on fish also requested at C.2. below (triggered by Annex VIII, Section 9.1.3., column 2)

Short-term toxicity testing on fish is a standard information requirement in Annex VIII to REACH (Annex VIII, Section 9.1.3). Long-term toxicity testing on fish must be considered (Section 9.1.3., Column 2) if the substance is poorly water soluble.

The Substance is poorly water soluble (<0.4 µg/L).

Therefore, long-term toxicity testing is needed to accurately define the hazard of the Substance.

The examination of the information provided, as well as the selection of the requested test and the test design are addressed in Appendix C, section 2.

ECHA has also adressed your comments to the draft decision in that section below.

2.-4. The soil simulation testing also requested at C.3., sediment simulation testing also requested at C.4., identification of degradation products also requested at C.5. (triggered by Annex VIII, Section 9.2., column 2)

Further degradation testing must be considered if the chemical safety assessment (CSA) according to Annex I indicates the need to investigate further the degradation of the substance (Annex VIII, Section 9.2., column 2).

Annex I, Section 4 requires that the CSA includes the PBT (persistent, bioaccumulative and toxic) and vPvB (very persistent and very bioaccumulative) assessments. In accordance with Annex XIII, Section 2.1., if the result of the screening tests or other information indicate that the substance may have PBT or vPvB properties, further testing on degradation as set out in Section 3.2 is required.

Screening information demonstrating potential PBT or vPvB properties include the following (ECHA Guidance R.11, Sections R.11.4 and Annex XIII):

- the substance is not readily biodegradable and thus potentially persistent; and
- the substance has high potential for bioaccumulation (log Kow > 4.5)

Screening information provided in your dossier indicates that the Substance may have PBT/vPvB properties:

- the Substance is potentially P/vP since it has not been demonstrated to be readily biodegradable (no data has been provided in the technical dossier that fulfil ready biodegradability criteria as expressed at OECD TG 301); and
- the Substance is potentially B/vB since the Log Kow is above the threshold of 4.5 (you estimated Log Kow of > 6.7)

The available screening information is not sufficient to conclude on the P/vP properties of the Substance, therefore further testing is required.

The trigger, the examination of the available information or adaptations, as well as the selection of the requested tests and the tests design are addressed respectively in Appendix C, Sections 3-5 below.

ECHA has also adressed your comments to the draft decision in Appendix C, Section 4 below.

5. Bioaccumulation in aquatic species also requested at C.6. below (triggered by Annex I, section 0.6.1 and 4. In conjunction with Annex XIII, Section 2.1.)

Bioaccumulation in aquatic species is required for the purpose of PBT/vPvB assessment (Annex I, Sections 0.6.1 and 4 to REACH).

Annex I, Section 4 requires that the CSA includes the PBT (persistent, bioaccumulative and toxic) and vPvB (very persistent and very bioaccumulative) assessments.

In accordance with Annex XIII, Section 2.1., if the result of the screening tests or other information indicate that the substance may have PBT or vPvB properties, further testing on bioaccumulation as set out in Section 3.2 is required.

As described above in Appendix B, Sections 2-4 above, screening information provided in your dossier indicates that the Substance may have PBT/vPvB properties. The available screening information is not sufficient to conclude on the B/vB properties of the Substance, and therefore further testing is required.

The trigger, the examination of the available information or adaptations, as well as the selection of the requested tests and the tests design are addressed respectively in in Appendix C, Section 6.

ECHA has also adressed your comments to the draft decision in that section below.

Appendix C: Reasons to request information required under Annex IX of REACH

1. Long-term toxicity testing on aquatic invertebrates (Annex IX, Section 9.1.5.)

Long-term toxicity testing on aquatic invertebrates is a standard information requirement of Annex IX of REACH.

You have sought to adapt this information requirement based on Annex IX, Section 9.1, Column 2.

We have assessed this information and identified the following issue(s).

Under Annex IX, Section 9.1, Column 2 of REACH, you must perform long-term toxicity testing on aquatic organisms unless your Chemical Safety Assessment (CSA) demonstrates that risks arising from the use of the Substance are controlled.

In particular, the Chemical Safety Assessment must take into account the following elements to support that long-term toxicity testing is not required:

- all relevant hazard information from your registration dossier,
- the outcome of the exposure assessment in relation to the uses of the Substance
- the outcome of the PBT/vPvB assessment including information on relevant degradation products and constituents present in concentration at or above 0.1% (w/w).

You have based your adaptation on the claim that: "*In view of its insolubility in water, its low bioaccumulating potential, its high molecular weight and the expected lack of effects in the acute aquatic studies (read across), the substance is concluded not be bioavailable to aquatic invertebrates to such an extent that it will cause adverse effects. Therefore, no long-term testing is proposed.*".

The Substance is poorly water soluble (<0.4 µg/L).

You have not provided experimental information on the bioavailability of the Substance itself.

For hydrophobic or poorly water soluble (e.g. water solubility below 1 mg/L or below the detection limit of the analytical method of the test substance), long-term tests must be considered (REACH Annex VII , Section 9.1.1, Column 2 and REACH Annex VIII , Section 9.1.3, Column 2), regardless of bioavailability. In any case, the information provided does not demonstrate the absence of bioavailability.

In your comments to the draft decision you stated that further information is available, providing a link to a GLP study performed according to OECD TG 211 (Daphnia magna Reproduction Test). Due to the limited information provided in this link , ECHA cannot make an independent assessment of the study (e.g. validity criteria, analytical monitoring, solvent concentration used, preparation of the concentration tested). In addition, you indicate that you will update your dossier. Please note that this decision does not take into account updates of the registration dossiers after the date on which you were notified of the draft decision according to Article 50(1) of REACH (see section 5.4. of ECHA's Practical Guide "How to act in Dossier Evaluation").

Therefore, your adaptation does not fulfil the information requirement.

Due to the low solubility of the substance in water you need to consult the OECD GD 23 and ECHA Guidance, Chapter R7b, Table R.7.8-3 relating to the aquatic toxicity testing of difficult substances, so that you choose the most appropriate design of the requested ecotoxicity test(s) and you best calculate and report the results of the test(s).

2. Long-term toxicity testing on fish (Annex IX, Section 9.1.6.1.)

Long-term toxicity testing on fish is a standard information requirement of Annex IX of REACH.

You have sought to adapt this information requirement based on Annex IX, Section 9.1 Column 2.

Your adaptation is rejected for the same reasons as explained in Appendix C.1 above.

In your comments to the draft decision you claim that Daphnia can be considered to be "*marginally more sensitive than fish in these types of tests*" and therefore that long-term toxicity test on fish is not necessary. To justify your claim, you have provided a link to a report entitled "Comparison of species sensitivity of Daphnia and fish in acute and chronic testing"[3]. ECHA has assessed this information against the requirement Annex IX, Section 9.1. The results and conclusions presented in the report are based on statistical observations, from a limited dataset. They are not substance-specific. In particular, the report explicitely warns that "*testing of both Daphnia and fish should be considered since no clear recommendation can be given based on the statistical result of this study. In the majority of cases (72 %) the chronic fish test is not necessary whereas 28 % of the substances are not properly covered by the chronic Daphnia test. Therefore, the chronic fish test should be considered unless substantial chronic fish toxicity can be excluded*". However, you have not provided, in your dossier or in your comments, any information that would rule out substantial chronic fish toxicity. Therefore, long term testing on fish must be performed.

In your comment to the draft decision you also make reference to ECHA Guidance R.7b indicating that further testing in fish is not required based on the assumption that acute tests in fish and both acute and chronic tests in Daphnia are available. As stated above in section C.1, as your Substance is poorly water soluble, acute studies cannot be used to assess the toxicity of the Substance. Therefore, long term testing must be performed.

Therefore, the information you have provided in your comments is not considered to fulfil the information requirement.

You must perform a long-term toxicity study on fish with the Substance.

Due to the low solubility of the substance in water you need to consult the OECD GD 23 and ECHA Guidance, Chapter R7b, Table R.7.8-3 relating to the aquatic toxicity testing of difficult substances, so that you choose the most appropriate design of the requested ecotoxicity test(s) and you best calculate and report the results of the test(s).

[3] Comparison of species sensitivity of Daphnia and fish in acute and chronic testing. TEXTE 87/2015. Environmental Research of the Federal Ministry for the Environment, Nature Conservation, Building and Nuclear Safety Project No. 27448 Report No. (UBA-FB) 002221/E, by Dr. Martin May, Dr. Stefan Hahn Fraunhofer-Institut für Toxikologie und Experimentelle Medizin (Fraunhofer ITEM), Hannover, Germany, on behalf of the German Environment Agency. ISSN 1862-4804, Dessau-Roßlau, October 2015. http://www.umweltbundesamt.de/publikationen/comparison-of-species-sensitivity-of-daphnia-fish

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

Soil simulation testing is a standard information requirement at Annex IX of REACH for substances with a high potential for adsorption to soil.

You have sought to adapt this information requirement based on Annex IX, Section 9.2.1.3, Column 2.

You justified the adaptation by stating that "*As the substance is not manufactured in Europe and at formulation or use waste is not disposed of via a waste water treatment plant, but incinerated, soil is not expected to be exposed. In accordance with REACH Annex IX, 9.2.1.3. the study need not be conducted if direct and indirect exposure of soil is unlikely.* "

We have assessed this information and identified the following issue(s):

Simulation testing on soil does not need to be conducted if direct or indirect exposure of soil is unlikely (Annex IX, Section 9.2.1.3, column 2).

Your dossier indicates the following uses: Environmental Release Category (ERC) 8a, 8d, 9a and 9b.

Based on the reported uses, soil exposure cannot be excluded and thus the absence of exposure has not been demonstrated.

Therefore, your adaptation does not fulfil the information requirement.

In your comments to the draft decision, you indicate your intention to perform a new ready biodegradability test with the Substance using one of the following methods: CO_2 Evolution test (OECD TG 301B) or Closed Bottle test (OECD TG 301D). If this new test shows that the Substance is readily biodegradable, then you will not perform the simulation studies and will not identify the degradation products requested under sections B 2 – 4 or C 3 – 5.

ECHA notes that you need not conduct the simulation tests and provide information on the identification of degradation products if the Substance is proven to be readily biodegradable (column 2 of Annex IX 9.2.1.3., 9.2.1.4. and 9.2.3.). Please note that this decision does not take into account updates of the registration dossiers after the date on which you were notified of the draft decision according to Article 50(1) of REACH (see section 5.4. of ECHA's Practical Guide "How to act in Dossier Evaluation)". ECHA will assess the information provided, including potential adaptations, after the set deadline of this decision for provision of the requested information passed.

Study design

Under Annex XIII, the information must be based on data obtained under conditions relevant for the PBT/vPvB assessment. Therefore:

- You must perform the test at the temperature of 12 °C, the average environmental temperature for the EU (ECHA Guidance R.16, Table R.16-8).
- Performing the tests at this temperature is in line with the applicable test conditions of the OECD TG 307.

Non-extractable residues (NER) must be quantified in all simulation studies. The reporting of results must include a scientific justification of the used extraction procedures and solvents. By default, total NER is regarded as non-degraded Substance. However, if reasonably justified and analytically demonstrated a certain part of NER may be differentiated and quantified as

irreversibly bound or as degraded to biogenic NER. Such fractions could be regarded as removed when calculating the degradation half-life(s) (ECHA Guidance Chapter R.11).

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

Sediment simulation testing is a standard information requirement at Annex IXIX of REACH for substances with a high potential for adsorption to sediment.

You have sought to adapt this information requirement based on Annex IX, Section 9.2.1.4, Column 2.

You justified the adaptation by stating that "*As it was concluded that the substance is not readily biodegradable, potential persistence has been confirmed and no further simulation testing is necessary. The substance is highly insoluble in ater, and in accordance with REACH Annex IX, 9.2.1.4. the study need not be conducted if direct and indirect exposure of sediment is unlikely.*"

We have assessed this information and identified the following issue(s):

A) Under REACH, there is no adaptation for the simulation testing on sediment based on low water solubility (Annex IX, Section 9.2.1.4, column 2; Annex XI).

B) Simulation testing on sediment does not need to be conducted if direct or indirect exposure of sediment is unlikely (Annex IX, Section 9.2.1.4, column 2).

Your dossier indicates the following uses: Environmental Release Category (ERC) 8a, 8d, 9a and 9b.

Based on the reported uses, soil exposure cannot be excluded and thus the absence of exposure has not been demonstrated

Therefore, your adaptation does not fulfil the information requirement.

ECHA has adressed your comments to the draft decision in section C.3 above.

Study design

The requested simulation tests shall be performed under relevant conditions (12°C) and non-extractable residues (NER) must be quantified, for the reasons explained above in Appendix C, Section 4.

5. Identification of degradation products (Annex IX, 9.2.3.)

You have not provided any information on 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.

We have assessed this information and identified the following issue(s).

Identity and relevance of degradation products must be included in the risk assessment and PBT assessment. Identification of degradation products does not need to be conducted if the substance is readily biodegradable (Annex IX, Section 9.2.3, column).

You have not provided information on identification of degradation products.

You have concluded the Substance as not readily biodegradable (IUCLID Section 5.2.1).

The Substance is not readily biodegradable. Information is needed for the PBT/vPvB assessment and risk assessment.

Therefore, the information provided does not fulfil the information requirement.

ECHA has adressed your comments to the draft decision in section C.3 above.

Study selection and design

You must obtain this information while performing the simulation studies requested in this decision (requests C.3 to C.5). You must provide a scientifically valid justification for any other method you have used for identification of the transformation/degradation products.

Identity, stability, behaviour, and molar quantity of the degradation/ transformation products relative to the Substance must be evaluated and reported, when analytically possible. In addition, degradation half-life, potential for bioaccumulation and toxicity of the transformation/degradation product must be investigated.

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

Bioaccumulation in aquatic species, preferably fish is a standard information requirement at Annex IX of REACH.

You have adapted the standard information requirement according to Annex XI, Section 1.2. Weight of evidence of REACH.

In support of your adaptation, you have provided the following sources of information:

(i) a QSAR prediction BCFBAF (v.4.0);
(ii) a QSAR prediction Toxicity Estimation Software Tool (T.E.S.T.) (v.4.1).

We have assessed this information and identified the following issue(s):

- Annex XI, Section 1.2 states that there may be sufficient weight of evidence from several independent sources of information leading to assumption/conclusion that a substance has or has not a particular dangerous (hazardous) property, while information from a single source alone is insufficient to support this notion.

According to ECHA Guidance R.4.4, a weight of evidence adaptation involves an assessment of the relative values/weights of different sources of information submitted. The weight given is based on the reliability of the data, consistency of results/data, nature and severity of effects, and relevance of the information for the given regulatory information requirement. Subsequently, relevance, reliability, consistency and results of these sources of information must be balanced in order to decide whether they together provide sufficient weight to conclude that the Substance has or has not the dangerous property investigated by the required study.

You have not included a justification for your WoE adaptation, which would include an assessment of relative weights of the individual pieces of information and the subsequent conclusions drawn.

Despite this critical deficiency, ECHA has assessed the information provided:

To fulfil the information requirement, normally a study according to OECD TG 305 must be provided. The key parameters investigated by this test are:

1) the uptake rate constant (k_1) and loss rate constants including the depuration rate constant (k_2), and/or
2) the steady-state bioconcentration factor (BCF_{SS}), and/or
3) the kinetic bioconcentration factor (BCF_K).

All the sources of information you provided investigate at least one key parameter. Therefore, they provide information that would contribute to the conclusion on this key parameter.

However, the reliability of these sources of information is significantly affected by the deficiencies identified below.

Annex XI, Section 1.3. states that results obtained from valid QSAR models may be used instead of testing when the following cumulative conditions are met, in particular:

1. results are derived from a QSAR model whose scientific validity has been established;
2. the substance falls within the applicability domain of the QSAR model; and
3. the results are adequate for classification and labelling and/or risk assessment.

i) Regarding the first estimation (BCFBAF v.4.0): the substance contains as a functional group 4 esters, 4 fragments of "linear C4 terminal chain and 4 fragments of -CH-, where the Maximum Number of each fragment in any Individual compound are 3, 2 and 2, respectively, for this model. Thus, the Substance does not fall within the applicability domain of the (Q)SAR model

ii) Regarding the second estimation (T.E.S.T., v.4.1): You state in IUCLID that *"this model includes strongly similar compounds with known experimental value in the training set and that the accuracy of prediction for similar molecules found in the training set is good."* However, no justification document is provided. Therefore, ECHA is not in a position to evaluate the (Q)SAR prediction and confirm that this model is suitable to predict properties of the Substance.

Therefore, the QSAR predictions are not considered reliable, because it can not be established whether the (Q)SAR models are scientifically valid and/or that the Substance falls within the applicability domain of the prediction models.

Taken together, even if these sources of information provide information on at least one key parameter, their reliability is affected so significantly that they cannot be taken into consideration in a weight of evidence approach.

Therefore, it is not possible to conclude, based on any source of information alone or considered together, whether your Substance has or has not the particular dangerous property foreseen to be investigated by the required study. Therefore, your adaptation is rejected.

In your comments to the draft decision you provided a link to a GLP study performed according to OECD TG 305 (Bioconcentration: Flow-through Fish Test). The information on this study is limited, but it appears that 2 test concentrations were used: 1 mg/L and 0.1 mg/L. Paragraph 24 of OECD TG 305 requires that the test concentrations for a flow-through fish test must be below the water solubility limit of the test substance for the test to be considered valid. The water solubility limit of the Substance as reported in your dossier is <0.4 µg/L at 20 °C. The

2 test concentrations of 1 mg/L and 0.1 mg/L are far above the water solubility limit of the Substance. Therefore, the study mentioned in your comments is likely not valid and would not fulfil the information requirement.

Therefore, the information requirement is not fulfilled.

Study design

Bioaccumulation in fish: aqueous and dietary exposure (test method EU C.13. / OECD TG 305) is the preferred test to investigate bioaccumulation (ECHA Guidance, Chapter R.7c, R.7.10.3.1, Chapter R.11). Whenever technically feasible, the aqueous route of exposure (OECD TG 305-I) must be used as the results obtained can be used directly for comparison with the B and vB criteria of Annex XIII of REACH. The low water solubility (0.4 µg/L) and the estimated high adsorption potential (log Kow > 6.7 and log Koc,soil >4.3) of the Substance indicate that conducting OECD TG 305 with aquatic exposure may be difficult. Therefore, in this case, the test is requested to be performed using dietary exposure. You must also attempt to estimate the corresponding BCF value from the dietary test (OECD 305-III) data according to Annex 8 of the OECD 305 TG and OECD Guidance Document on Aspects of OECD TG 305 on Fish Bioaccumulation, ENV/JM/MONO (2017)16. In any case you must report all data derived from the dietary test as listed in the OECD TG 305-III.

Appendix E: Requirements to fulfil when conducting and reporting new tests for REACH purposes

A. Test methods, GLP requirements and reporting

1. Under Article 13(3) of REACH, all new data generated as a result of this decision must be conducted according to the test methods laid down in a European Commission Regulation or to international test methods recognised by the Commission or ECHA as being appropriate.

2. Under Article 13(4) of REACH, ecotoxicological and toxicological tests and analyses must be carried out according to the GLP principles (Directive 2004/10/EC) or other international standards recognised by the Commission or ECHA.

3. Under Article 10(a)(vi) and (vii) of REACH, all new data generated as a result of this decision must be reported as study summaries, or as robust study summaries, if required under Annex I of REACH. See ECHA Practical Guide on How to report robust study summaries[4].

B. Test material

Before generating new data, you must agree within the joint submission on the chemical composition of the material to be tested (Test Material) which must be relevant for all the registrants of the Substance.

1. Selection of the Test material(s)
   The Test Material used to generate the new data must be selected taking into account the following:
   - the variation in compositions reported by all members of the joint submission,
   - the boundary composition(s) of the Substance,
   - the impact of each constituent/ impurity on the test results for the endpoint to be assessed. For example, if a constituent/ impurity of the Substance is known to have an impact on (eco)toxicity, the selected Test Material must contain that constituent/ impurity.

2. Information on the Test Material needed in the updated dossier
   - You must report the composition of the Test Material selected for each study, under the "Test material information" section, for each respective endpoint study record in IUCLID.
   - The reported composition must include all constituents of each Test Material and their concentration values and other parameters relevant for the property to be tested.

This information is needed to assess whether the Test Material is relevant for the Substance and whether it is suitable for use by all members of the joint submission.

Technical instructions on how to report the above is available in the manual on How to prepare registration and PPORD dossiers[5].

[4] https://echa.europa.eu/practical-guides
[5] https://echa.europa.eu/manuals

Appendix F: General recommendations when conducting and reporting new tests for REACH purposes

A. Strategy for the PBT/vPvB assessment

You are advised to consult ECHA Guidance R.7b (Section R.7.9.), R.7c (Section R.7.10) and R.11 on PBT assessment to determine the sequence of the tests needed to reach the conclusion on PBT/vPvB. The guidance provides advice on 1) integrated testing strategies (ITS) for the P, B and T assessments and 2) the interpretation of results in concluding whether the Substance fulfils the PBT/vPvB criteria of Annex XIII.

In particular, you are advised to first conclude whether the Substance fulfils the Annex XIII criteria for P and vP, and then continue with the assessment for bioaccumulation. When determining the sequence of simulation degradation testing you are advised to consider the intrinsic properties of the Substance, its identified uses and release patterns as these could significantly influence the environmental fate of the Substance. You must revise your PBT assessment when the new information is available.

Appendix G: Procedure

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

ECHA followed the procedure detailed in Articles 50 and 51 of REACH.

The compliance check was initiated on 21 May 2019.

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

ECHA took into account your comments and the change of the highest tonnage band and amended the request(s).

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

As no amendments were proposed, ECHA adopted the decision under Article 51(3) of REACH.

Appendix H: List of references - ECHA Guidance[6] and other supporting documents

Evaluation of available information
Guidance on information requirements and chemical safety assessment, Chapter R.4 (version 1.1., December 2011), referred to as ECHA Guidance R.4 where relevant.

QSARs, read-across and grouping
Guidance on information requirements and chemical safety assessment, Chapter R.6 (version 1.0, May 2008), referred to as ECHA Guidance R.6 where relevant.

Read-across assessment framework (RAAF, March 2017)[7]

RAAF - considerations on multiconstituent substances and UVCBs (RAAF UVCB, March 2017)[6]

Physical-chemical properties
Guidance on information requirements and chemical safety assessment, Chapter R.7a (version 6.0, July 2017), referred to as ECHA Guidance R.7a in this decision.

Toxicology
Guidance on information requirements and chemical safety assessment, Chapter R.7a (version 6.0, July 2017), referred to as ECHA Guidance R.7a in this decision.

Guidance on information requirements and chemical safety assessment, Chapter R.7c (version 3.0, June 2017), referred to as ECHA Guidance R.7c in this decision.

Environmental toxicology and fate
Guidance on information requirements and chemical safety assessment, Chapter R.7a (version 6.0, July 2017), referred to as ECHA Guidance R.7a in this decision.

Guidance on information requirements and chemical safety assessment, Chapter R.7b (version 4.0, June 2017), referred to as ECHA Guidance R.7b in this decision.

Guidance on information requirements and chemical safety assessment, Chapter R.7c (version 3.0, June 2017), referred to as ECHA Guidance R.7c in this decision.

PBT assessment
Guidance on information requirements and chemical safety assessment, Chapter R.11 (version 3.0, June 2017), referred to as ECHA Guidance R.11 in this decision.

Guidance on information requirements and chemical safety assessment, Chapter R.16 (version 3.0, February 2016), referred to as ECHA Guidance R.16 in this decision.

Data sharing
Guidance on data-sharing (version 3.1, January 2017), referred to as ECHA Guidance on data sharing in this decision.

OECD Guidance documents[8]

[6] https://echa.europa.eu/guidance-documents/guidance-on-information-requirements-and-chemical-safety-assessment
[7] https://echa.europa.eu/support/registration/how-to-avoid-unnecessary-testing-on-animals/grouping-of-substances-and-read-across
[8] http://www.oecd.org/chemicalsafety/testing/series-testing-assessment-publications-number.htm

Guidance Document on aqueous-phase aquatic toxicity testing of difficult test chemicals – No 23, referred to as OECD GD 23.

Guidance document on transformation/dissolution of metals and metal compounds in aqueous media – No 29, referred to as OECD GD 29.

Guidance Document on Standardised Test Guidelines for Evaluating Chemicals for Endocrine Disruption – No 150, referred to as OECD GD 150.

Guidance Document supporting OECD test guideline 443 on the extended one-generation reproductive toxicity test – No 151, referred to as OECD GD 151.

Appendix I: List of the registrants to which the decision is addressed and the corresponding information requirements applicable to them

Registrant Name	Registration number	(Highest) Data requirements to be fufilled
[redacted]	[redacted]	[redacted]
[redacted]	[redacted]	[redacted]
[redacted]	[redacted]	[redacted]
[redacted]	[redacted]	[redacted]
[redacted]	[redacted]	[redacted]
[redacted]	[redacted]	[redacted]
[redacted]	[redacted]	[redacted]
[redacted]	[redacted]	[redacted]

Note: where applicable, the name of a third party representative (TPR) may be displayed in the list of recipients whereas the decision is sent to the actual registrant.