~~Confidential~~

Helsinki, 01 September 2023

Addressee(s)
Registrant(s) of DPP Reg Dossier as listed in Appendix 3 of this decision

Date of submission of the dossier subject to this decision
12 July 2022

Registered substance subject to this decision ("the Substance")
Substance name: diphenyl phosphonate
EC number/List number: 225-202-8

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 information listed below by ***9 December 2024***.

Requested information must be generated using the Substance unless otherwise specified.

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

1. Short-term toxicity testing on aquatic invertebrates (Annex VII, Section 9.1.1.; test method: EU C.2./OECD TG 202)

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

3. Ready biodegradability (Annex VII, Section 9.2.1.1.; test method: EU C.4. A/B/C/D/E/F/OECD TG 301A/B/C/D/E/F or EU C.29./OECD TG 310)

The reasons for the request(s) are explained in Appendix 1.

Information required depends on your tonnage band

You must provide the information listed above for all REACH Annexes applicable to you in accordance with Articles 10(a) and 12(1) of REACH. The addressees of the decision and their corresponding information requirements based on registered tonnage band are listed in Appendix 3.

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

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 requirements for testing and reporting new tests under

REACH, see Appendix 4.

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 Mike Rasenberg, Director of Hazard Assessment

Appendix 1: Reasons for the request(s)
Appendix 2: Procedure
Appendix 3: Addressees of the decision and their individual information requirements
Appendix 4: Conducting and reporting new tests under REACH

[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 1: Reasons for the request(s)

Contents

Reasons related to the information under Annex VII of REACH

1. Short-term toxicity testing on aquatic invertebrates

1 Short-term toxicity testing on aquatic invertebrates is an information requirement under Annex VII to REACH (Section 9.1.1.).

1.1. Information provided

2 You have adapted this information requirement by using Qualitative or Quantitative Structure-Activity Relationships ((Q)SARs). To support the adaptation, you have provided the following information:

(i) a prediction from QSAR with ECOSAR Ester class (v.1.1), 2022.

1.2. Assessment of the information provided

1.2.1. QSAR adaptation rejected

3 Under Annex XI, Section 1.3., the following condition, among others, must be fulfilled whenever a (Q)SAR approach is used:

(1) results need to be adequate for the purpose of risk assessment or classification and labelling

4 With regard to this condition, we have identified the following issue(s):

1.2.1.1. The prediction does not cover all components of the Substance

5 Under Guidance on IRs and CSA R.6.1.7.3. a prediction is adequate for the purpose of classification and labelling and/or risk assessment if the following conditions are met:

- the composition of the substance is clearly defined, and
- different constituents or components of the same substance are predicted individually.

6 Your registration dossier provides the following information:

- According to the documentation "[redacted]" submitted in the registration dossier, you provided predictions for the following structures: diphenyl phosphonate (SMILES : O=P(Oc1ccccc1)(Oc2ccccc2))

7 Your substance has tautomerism, containing two components "diphenyl phosphonate" (the P(V) form) and "diphenyl phosphite" (the P(III) form) which exist in equilibrium in the Substance.

8 You have provided the prediction only for one tautomer (diphenyl phosphonate), and the diphenyl phosphite tautomer (SMILE: OP(Oc1ccccc1)Oc1ccccc1) has not been covered by the prediction. You have not covered all relevant components of the Substance.

9 Therefore, you have not demonstrated that the prediction is adequate for the purpose of classification and labelling and/or risk assessment.

1.2.1.2. The prediction is not adequate due to low reliability

10 Under ECHA Guidance R.6.1.3.4. a prediction is adequate for the purpose of classification and labelling and/or risk assessment when the model is applicable to the chemical of interest with the necessary level of reliability. ECHA Guidance R.6.1.5.3. specifies that, among others, the following condition must be met:

- the model predicts well substances that are similar to the substance of interest

11 Your registration dossier provides the following information:

- predictions from the ECOSAR v.1.11 model for Esters class without information on close analogues

12 Based on the publicly available information on the model, the model for Esters class does not contain phosphonate substances in the training set of the short-term Daphnia model. Hence, you have not demonstrated that model predicts well substances that are similar to the Substance and the predicted values cannot be considered reliable.

13 Therefore, you have not demonstrated that the prediction for the Substance is adequate for the purpose of classification and labelling and/or risk assessment.

14 Based on the above, your QSAR adaptation under Annex XI, Section 1.3. is rejected.

1.3. Assessment of your comments to the draft decision

15 In your comments to the draft decision, you do not agree to perform the requested study. You state that it is not feasible to test the Substance (DPP) in aquatic test system due to hydrolysis to phenol and phosphorous acid. In addition, you claim that hydrolysis for DPP is expected to be faster than the source substance (TPP), for which there is hydrolysis data available in the dossier. You present the following two options to address short-term toxicity to aquatic invertebrates:

(1) "*Use aquatic toxicity data on phenol to address the environmental endpoints. This would include the classification of Aquatic Chronic 2 (H411).*"

(2) "*Use the ECOSAR data for OP(Oc1ccccc1)(Oc2ccccc2) and classify the substance as Aquatic Acute 1 (H400).*"

16 Regarding option 2, as explained above, the QSAR adaptation under Annex XI, Section 1.3. is rejected. In your comments you agree that "…*the validity of the model for this substance is uncertain*" but you have not provided any further justification that would adress the reliability issues related to the prediction as identified above.

17 Regarding option 1, while you have not identified this information as a read-across adaptation, since phenol is a different substance than the Substance, ECHA understands that you intend to rely on a read-across adaptation under Annex XI, Section 1.5 of REACH.

18 In this regard, while you present a read-across strategy intending to rely on aquatic toxicity data on phenol ('source substance'), you do not provide any supporting information regarding your read-across hypothesis or robust study summaries of studies conducted on the source substance.

19 As your read-across strategy relies on a read-across approach that has not yet been fully justified, as well as on data which is not yet provided in your comments or your dossier, no conclusion on the compliance of your proposed adaptation can be made.

20 Additional information on what is necessary when justifying a read-across approach can be found in the Guidance on IRs and CSA, Chapter R.6. and related documents (RAAF, 2017; RAAF UVCB, 2017). The documentation provided needs to be sufficient to allow an independent scientific assessment. The ECHA Guidance lists the elements that need to be included in the documentation of read-across approaches.

21 You remain responsible for complying with this decision by the set deadline.

22 Therefore, the information requirement is not fulfilled.

1.4. Study design and test specifications

23 You indicate that the Substance is difficult to test with the following statement in your dossier: "Based on experiences with attempting to design and conduct appropriate studies to investigate the ecotoxicity of alkyl and aryl phosphites, it was determined that conducting aquatic toxicity studies on diphenyl phosphonate (DPP) in algae, daphnia and fish would not be possible. This conclusion is consistent with OECD Guidance Document #23 entitled "Guidance Document on Aquatic Toxicity Testing of Difficult Substances and Mixtures" (OECD 2000) because of the inherent physical/chemical properties of the test substance (i.e. poor water solubility and hydrolysis)." OECD TG 202 specifies that, for difficult to test substances, you must consider the approach described in OECD GD 23 or other approaches, if more appropriate for your substance. In all cases, the approach selected must be justified and documented.

24 If the Substance hydrolyses rapidly in the test system, aquatic toxicity of hydrolysis degradation products may be determined by allowing the parent compound to degrade and then exposing the test organisms to the resulting test solution. The decision to test the parent test chemical and/or its degradation products must be based on a consideration of its half-life.

25 Due to the properties of Substance, it may be difficult to achieve and maintain the desired exposure concentrations. Therefore, you must monitor the test concentration(s) of the Substance or its hydrolysis products (depending on the rate of hydrolysis and/or the relative (eco)toxicities of the parent test chemical and degradation products) throughout the exposure duration and report the results. If it is not possible to demonstrate the stability of exposure concentrations (i.e. measured concentration(s) not within 80-120% of the nominal concentration(s)), you must express the effect concentration based on measured values as described in OECD TG 202. In case a dose-response relationship cannot be established (no observed effects), you must demonstrate that the approach used to prepare test solutions was adequate to maximise the concentration of the Substance, or the hydrolysis product(s) in the test solution.

2. Growth inhibition study aquatic plants

26 Growth inhibition study on aquatic plants is an information requirement under Annex VII to REACH (Section 9.1.2.).

2.1. Information provided

27 You have adapted this information requirement by using Qualitative or Quantitative Structure-Activity Relationships ((Q)SARs). To support the adaptation, you have provided the following information:

(i) a prediction from QSAR with ECOSAR Ester class (v.1.1), 2022.

2.2. Assessment of the information provided

2.2.1. QSAR adaptation rejected

28 Under Annex XI, Section 1.3., the following condition, among others, must be fulfilled whenever a (Q)SAR approach is used:

(2) results need to be adequate for the purpose of risk assessment or classification and labelling

29 With regard to this condition, we have identified the following issue(s):

2.2.1.1. The prediction does not cover all components of the Substance

30 Under Guidance on IRs and CSA R.6.1.7.3. a prediction is adequate for the purpose of classification and labelling and/or risk assessment if the following conditions are met:

- the composition of the substance is clearly defined, and
- different constituents or components of the same substance are predicted individually.

31 Your registration dossier provides the following information:

- According to the documentation "[redacted]" submitted in the registration dossier, you provided predictions for the following structures: diphenyl phosphonate (SMILES : O=P(Oc1ccccc1)(Oc2ccccc2))

32 Your substance has tautomerism, containing two components "diphenyl phosphonate" (the P(V) form) and "diphenyl phosphite" (the P(III) form) which exist in equilibrium in the Substance.

33 You have provided the prediction only for one tautomer (diphenyl phosphonate), and the diphenyl phosphite tautomer (SMILE: OP(Oc1ccccc1)Oc1ccccc1) has not been covered by the prediction. You have not covered all relevant components of the Substance.

34 Therefore, you have not demonstrated that the prediction is adequate for the purpose of classification and labelling and/or risk assessment.

2.2.1.2. The prediction is not adequate due to low reliability

35 Under ECHA Guidance R.6.1.3.4. a prediction is adequate for the purpose of classification and labelling and/or risk assessment when the model is applicable to the chemical of interest with the necessary level of reliability. ECHA Guidance R.6.1.5.3. specifies that, among others, the following condition must be met:

- the model predicts well substances that are similar to the substance of interest

36 Your registration dossier provides the following information:

- predictions from the ECOSAR v.1.11 model for Esters class without information on close analogues

37 Based on the publicly available information on the model, the model for Esters class does not contain phosphonate substances in the training set of the algae model. Hence, you have not demonstrated that model predicts well substances that are similar to the Substance and the predicted values cannot be considered reliable.

38 Therefore, you have not demonstrated that the prediction for the Substance is adequate for the purpose of classification and labelling and/or risk assessment.

39 Based on the above, your QSAR adaptation under Annex XI, Section 1.3. is rejected.

2.3. Assessment of your comments to the draft decision

40 In your comments to the draft decision, you provide the same information for growth inhibition study on aquatic plants as for the short-term toxicity to aquatic invertebrates, presented under Section 1.3.

41 As explained under Section 1.3, no conclusion on the compliance of the proposed adaptation can be made.

42 Therefore, the information requirement is not fulfilled. You remain responsible for complying with this decision by the set deadline.

2.4. Study design and test specifications

43 OECD TG 201 specifies that, for difficult to test substances, OECD GD 23 must be followed. As already explained above, the Substance is difficult to test. Therefore, you must fulfil the requirements described in 'Study design and test specifications' under request 1.

3. Ready biodegradability

44 Ready biodegradability is an information requirement in Annex VII to REACH (Section 9.2.1.1.).

3.1. Information provided

45 You have adapted this information requirement by using Annex XI, Section 1.5. (Grouping of substances and read-across approach) based on the following experimental data:

(i) a ready biodegradability study (2015) with the source substance TRIPHENYL PHOSPHITE, EC 202-908-4 (TPP)

3.2. Assessment of the information provided

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

3.2.1. Read-across adaptation rejected

47 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.

48 Additional information on what is necessary when justifying a read-across approach can be found in the Guidance on IRs and CSA, Chapter R.6. and related documents (RAAF, 2017; RAAF UVCB, 2017).

49 You provide the following reasoning for the prediction of this information requirement: "Diphenyl phosphonate (DPP) is expected to have similar chemical properties to that of triphenyl phosphite (TPP), which is a structurally similar compound and minor constituent in DPP. This relationship is explained more fully in the paper attached in Section 13 of this dossier."

50 However, a read-across justification document in IUCLID Section 13.2 to which you refer, does not provide any reasoning for the degradation property.

51 We have identified the following issue(s) with the prediction of (eco)toxicological / environmental fate properties:

3.2.1.1. Lack of read-across hypothesis for biodegradation properties

52 Annex XI, Section 1.5. requires that whenever read-across is used adequate and reliable documentation of the applied method must be provided. Such documentation must include an information requirement specific explanation why the properties of the Substance may be predicted from other substances in the group, i.e. a read-across hypothesis. This hypothesis should be based on recognition of the structural similarities and differences between the substances (Guidance on IRs and CSA, Section R.6.). It should explain why the differences in the chemical structures should not influence the biodegradation properties or should do so in a regular pattern.

53 You have not provided any read-across justification document covering this information requirement.

54 In addition ECHA notes that your general statement regarding structural similarity between the source substance and the Substance, which you consider a sufficient basis for predicting the properties of the Substance, is not adequate.

55 While structural similarity is a prerequisite for applying the grouping and read-across approach, it does not necessarily lead to predictable or similar (eco)toxicological / environmental fate properties. You have not provided a well-founded hypothesis to establish a reliable prediction for biodegradation property.

56 As explained above, you have not established that relevant properties of the Substance can be predicted from data on the source substance. On this basis, your read-across approach under Annex XI, Section 1.5. is rejected.

3.3. Assessment of your comments to the draft decision

57 In your comments to the draft decision, you do not agree to perform the requested study. You state that "*Based on the chemical relationship between DPP and TPP, PSRC believes that DPP will be as or more biodegradable than TPP. The expected environmental transformation pathway for both DPP and TPP is hydrolysis to phenol followed by the microbial biodegradation of the phenol.*" You state that TPP and phenol are readily biodegradable. Based on this, you conclude that the read-across adaptation based on data conducted on TPP is appropriate for this information requirement.

58 ECHA acknowledges your intention to further improve your read-across hypothesis for this information requirement. However, you provide very limited information to support your read-across adaptation. More specifically, you have not addressed the following issue identified above, i.e. explanation of why the differences in the chemical structures between the Substance and the source substance should not influence the biodegradation properties of the Substance.

59 You can find additional guidance on how to apply a read-across approach in the Guidance on IRs and CSA, Chapter R.6. and related documents (RAAF, 2017; RAAF UVCB, 2017). As explained in the read-across assessment framework (RAAF, 2017), the read-across approach must be justified scientifically and documented thoroughly, also taking into account the differences in the chemical structures of the substances. There may be several lines of supporting evidence used to justify the read-across hypothesis with the aim of strengthening the latter.

60 In addition, you have not updated the read-across justification in your registration dossier regarding this information requirement. Therefore, the information provided in your

comments does not change the assessment outcome. Therefore, the information requirement is not fulfilled and the data gap remains.

61 You remain responsible for complying with this decision by the set deadline.

References

The following documents may have been cited in the decision.

Guidance on information requirements and chemical safety assessment (Guidance on IRs & CSA)

Chapter R.4 Evaluation of available information; ECHA (2011).
Chapter R.6 QSARs, read-across and grouping; ECHA (2008).
Appendix to Chapter R.6 for nanoforms; ECHA (2019).
Chapter R.7a Endpoint specific guidance, Sections R.7.1 – R.7.7; ECHA (2017).
Appendix to Chapter R.7a for nanomaterials; ECHA (2017).
Chapter R.7b Endpoint specific guidance, Sections R.7.8 – R.7.9; ECHA (2017).
Appendix to Chapter R.7b for nanomaterials; ECHA (2017).
Chapter R.7c Endpoint specific guidance, Sections R.7.10 – R.7.13; ECHA (2017).
Appendix to Chapter R.7a for nanomaterials; ECHA (2017).
Appendix R.7.13-2 Environmental risk assessment for metals and metal compounds; ECHA (2008).
Chapter R.11 PBT/vPvB assessment; ECHA (2017).
Chapter R.16 Environmental exposure assessment; ECHA (2016).

Guidance on data-sharing; ECHA (2017).
Guidance for monomers and polymers; ECHA (2012).
Guidance on intermediates; ECHA (2010).
All guidance documents are available online: https://echa.europa.eu/guidance-documents/guidance-on-reach

Read-across assessment framework (RAAF)

RAAF, 2017 Read-across assessment framework (RAAF); ECHA (2017).
RAAF UVCB, 2017 Read-across assessment framework (RAAF) – considerations on multi- constituent substances and UVCBs; ECHA (2017).

The RAAF and related documents are available online:
https://echa.europa.eu/support/registration/how-to-avoid-unnecessary-testing-on-animals/grouping-of-substances-and-read-across

***OECD Guidance documents* (OECD GDs)**

OECD GD 23 Guidance document on aquatic toxicity testing of difficult substances and mixtures; No. 23 in the OECD series on testing and assessment, OECD (2019).
OECD GD 29 Guidance document on transformation/dissolution of metals and metal compounds in aqueous media; No. 29 in the OECD series on testing and assessment, OECD (2002).
OECD GD 150 Revised guidance document 150 on standardised test guidelines for evaluating chemicals for endocrine disruption; No. 150 in the OECD series on testing and assessment, OECD (2018).
OECD GD 151 Guidance document supporting OECD test guideline 443 on the extended one-generation reproductive toxicity test; No. 151 in the OECD series on testing and assessment, OECD (2013).

Appendix 2: 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 2 May 2022.

The deadline of the decision is set based on standard practice for carrying out OECD TG tests. It has been exceptionally extended by 6 months from the standard deadline granted by ECHA to take into account currently longer lead times in contract research organisations.

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

ECHA took into account your comments and did not amend 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 3: Addressee(s) of this decision and their corresponding information requirements

In accordance with Articles 10(a) and 12(1) of REACH, the information requirements for individual registrations are defined as follows:

- 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;

Registrant Name	Registration number	Highest REACH Annex applicable to you
[redacted]	[redacted]	[redacted]
[redacted]	[redacted]	[redacted]
[redacted]	[redacted]	[redacted]

Where applicable, the name of a third party representative (TPR) may be displayed in the list of recipients whereas ECHA will send the decision to the actual registrant.

Appendix 4: Conducting and reporting new tests for REACH purposes

1. Requirements when conducting and reporting new tests for REACH purposes

1.1. 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[2].

(4) Under the introductory part of Annexes VII/VIII/IX/X to REACH, where a test method offers flexibility in the study design, for example in relation to the choice of dose levels or concentrations, the chosen study design must ensure that the data generated are adequate for hazard identification and risk assessment.

1.2. 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

[2] https://echa.europa.eu/practical-guides

With that detailed information, ECHA can confirm 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 (https://echa.europa.eu/manuals).