Helsinki, 29 March 2023

Addressee
Registrant of 2,5-di-tert-pentylhydroquinone listed in the last Appendix of this decision

Registered substance subject to this decision (the Substance)
Substance name: 2,5-di-tert-pentylhydroquinone (DAHQ)
EC number: 201-222-2
CAS number: 79-74-3

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

DECISION ON SUBSTANCE EVALUATION

Under Article 46 of Regulation (EC) No 1907/2006 (REACH), you must submit the information listed below.

A. The information required is to be generated on [redacted], a relevant transformation product of the Substance, to clarify the potential risk related to PBT/vPvB:

1. Vapour pressure (test method: EU A.4/OECD TG 104).

2. Determination of Henry's law constant (HLC) using one of the experimental approaches defined within Appendix R.7.1-1 of ECHA's Guidance[1]:
   - If you can demonstrate with documentary evidence that no suitable testing laboratory is available to conduct experimental measurements, the HLC may be calculated using the ratio of water solubility (c_w) to vapour pressure (vp) prediction approach defined in appendix R.7.1-1 of ECHA's Guidance.
   - You must provide an adequate justification for the calculation performed.

3. Water solubility (test method: EU A.6/OECD TG 105).

4. Partition Coefficient 1-Octanol/Water (test method: Slow-Stirring Method, OECD TG 123).

Deadline

The information must be submitted by **05 April 2024**.

Conditions to comply with the information requested

To comply with this decision, you must submit the information in an updated registration dossier, by the deadline indicated above. The information must comply with the IUCLID robust study summary format. You must also attach the full study report for the corresponding studies in the corresponding endpoint of IUCLID.

You must update the chemical safety report, where relevant, including any changes to classification and labelling, based on the newly generated information.

[1] ECHA's Guidance on Information Requirements and Chemical Safety Assessment, Chapter R.7a: Endpoint specific guidance (version 6.0, July 2017).

You will find the justifications for the requests in this decision in the Appendix entitled ''Reasons to request information to clarify the potential risk.'

You will find the procedural steps followed to reach the adopted decision and some technical guidance detailed in further Appendices.

Appeal

This decision 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[2] by Mike Rasenberg, Director of Hazard Assessment

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

Basis for substance evaluation

The objective of substance evaluation under REACH is to allow for the generation of further information on substances suspected of posing a risk to human health or the environment ('potential risk').

ECHA has concluded that further information on the Substance is necessary to enable the evaluating Member State Competent Authority (MSCA) to clarify a potential risk and whether regulatory risk management is required to ensure the safe use of the Substance.

The ECHA decision requesting further information is based on the following:

(1) There is a potential risk to human health and/ or the environment, based on a combination of hazard and exposure information.
(2) Information is necessary to clarify the potential risk identified; and
(3) There is a realistic possibility that the information requested would allow improved risk management measures to be taken.

The Appendices entitled 'Reasons to request information' describe why the requested information are necessary and appropriate.

Appendix A – Reasons to request information to clarify the potential risk related to PBT/vPvB

After the evaluation of all requested and relevant information submitted on 2,5-di-tert-pentylhydroquinone because of a first evaluation step, the evaluating MSCA concluded that further information is still required to complete the evaluation of whether the Substance constitutes a risk to the environment.

A relevant transformation product of the Substance, [redacted], has potential PBT/vPvB properties and is also an impurity of the Substance with a typical concentration > 0.1%.

Annex XIII of REACH provides that the identification of PBT/vPvB substances must also consider the PBT/vPvB properties of relevant transformation and/or degradation products. If a fraction/specific constituent of UVCB/multi-constituent substances and/or degradation/transformation products show PBT/vPvB properties, the parent substance is identified as PBT/vPvB.

Therefore, further information is needed on [redacted] to clarify if the transformation product, and hence the Substance, have PBT/vPvB properties.

Once the results from the tests requested in this decision are available, the evaluating MSCA will be able to decide on the need for further information to examine the potential PBT/vPvB hazards of the transformation products.

1. Potential risk

1.1 Potential hazard of the Substance

Following its assessment of the available relevant information on the Substance, the evaluating MSCA has identified the following potential hazard(s) which must be clarified.

a) Potential P/vP properties

The available information suggests that the Substance may have P/vP properties.

Following the request in the first Substance Evaluation decision, and since the log K_{ow} of the Substance has been determined to be greater than 4.5, you submitted a simulation test on ultimate degradation in surface water, performed with the Substance (OECD TG 309; Aerobic Mineralisation in Surface Water - Simulation Biodegradation Test).

Since the water solubility of the Substance is very low (< 0.2 µg/L, measured according to OECD TG 105), acetonitrile was used to dissolve the Substance and to prepare spiked solutions, which were used to treat the water phase to obtain concentrations of ^{14}C-labeled DAHQ of ~10 and ~100 µg/L. The study showed that the Substance did not undergo mineralization since NaOH traps did not register any relevant formation of CO_2. The Substance quickly dissipated in the surface water to less than 10% of applied radioactivity within 7 days of incubation in the test systems treated at a low-test concentration (10 µg/L) and within 11 days of incubation in the test systems treated at a high-test concentration (100 µg/L). One relevant transformation product, identified as [redacted], formed in water simultaneously with the disappearance of the Substance.

The concentration of [redacted] rapidly decreased in water and increased in polyurethane foam (PUF) traps, indicating that [redacted] dissipated from water due to volatilization ([redacted]% at low

test concentration and [redacted]% at high test concentration in PUFs, at the end of the study). The disappearance of the Substance in water resulted from quick oxidation in the equivalent quinone, as confirmed even by the sterile controls and to volatilization, as demonstrated by the presence in the PUF traps ([redacted]% at low test concentration and [redacted]% at high test concentration at the end of the study). In conclusion, abiotic transformation is the main degradation route and volatilization the main dissipation route of the Substance in the water compartment.

Therefore, the DT_{50} values presented in the study would be associated to a primary degradation and disappearance from the water compartment, and not to a mineralization. High dissipation due to volatilization, reversibility of oxidation and concentrations above the water solubility, which could result in a lack of bioavailability by microorganisms, do not allow to conclude whether the Substance is P when comparing to the criteria of Annex XIII of REACH.

Moreover, you provided QSAR predictions for [redacted], identified also as an impurity of the Substance. You concluded that [redacted] is 'not biodegradable' and is potential vP (and P) on a worst-case basis. Using BIOWIN™ v4.10, the evaluating MSCA estimates the following biodegradability parameters for [redacted]:

BIOWIN 1 - linear biodegradation prediction: 0.2751 (does not biodegrade fast)
BIOWIN 2 - non-linear biodegradation prediction: 0.0076 (does not biodegrade fast)
BIOWIN 3 - survey model ultimate biodegradation timeframe: 2.1811 (≥ weeks - month)
BIOWIN 4 - survey model primary biodegradation timeframe: 3.1381 (≥ days - weeks)
BIOWIN 5 - MITI linear biodegradation prediction: 0.4576 (not readily degradable)
BIOWIN 6 - MITI non-linear biodegradation prediction: 0.2410 (not readily degradable)
BIOWIN 7 - Anaerobic model prediction: -1.1887 (does not biodegrade fast)

Based on the above predictions, the evaluating MSCA identifies the transformation product, [redacted], as potential vP (and P).

The available and current information is not sufficient to draw a conclusion on the hazard. Further information is needed on the physicochemical properties of [redacted], which you identified as the relevant transformation product of the Substance in the water compartment.

b) Potential B/vB properties

The available information suggest that the Substance may have B/vB properties

In the updated dossier you identified [redacted] as the relevant transformation product.

The evaluating MSCA considers the following:

- For the Substance: you provided new partition coefficient studies, measured in a GLP OECD TG 123 study (slow-stirring method). The slow-stirring method is particularly suitable for substances with log K_{ow} values >5 and was therefore considered appropriate for highly hydrophobic substances such as DAHQ. The log K_{ow} values from the slow-stirring method results (> 4.5) indicated a potential bioaccumulative behavior for the Substance.

- For the transformation product, [redacted]: you assessed it as not B (vB) based on a BCF value <=2000 L/kg.

Based on results of the QSAR model, BCFBAF v3.01, [redacted] does not screen as "B" with:
- BCF =537.7 L/kg (w/w) and BAF = 543.6 L/kg (w/w) for upper trophic.
- BCF = 703.5 L/kg (w/w) and BAF = 774.9 L/kg (w/w) for mid trophic.
- BCF = 757.4 L/kg (w/w) and BAF = 1042 L/kg (w/w) for lower trophic.

It is noted that the above values are derived including biotransformation rate estimates. If a zero-biotransformation rate is assumed, then BCF = 8536 (upper trophic). Moreover, EPISUITE v4.10 predicts a log K_{ow} for [redacted]=5.05, that indicates a potential B/vB property.

c) Potential T properties

As stated above, according to QSAR predictions, ECHA considers that the transformation product, [redacted], screens as P/vP and B/vB. Moreover, you assessed [redacted] as potential T based on Ecotox QSAR, although you did not specify the predicted values.

Using ECOSAR v1.11, the evaluating MSCA predicts for [redacted] a fish 96h LC_{50} = 0.021 mg/L, a daphnid 48h LC_{50} = 0.030 mg/L and a green algae EC_{50} = 0.036 mg/L. Overall, ECHA agrees in identifying [redacted] as potential T.

The available and current information is not sufficient to draw a conclusion on the hazard posed by the Substance. Further information is needed on the physicochemical properties of [redacted], which you identified as the relevant transformation product of DAHQ in the water compartment.

1.2 Potential exposure

According to the information you submitted in all registration dossiers and chemical safety reports, the aggregated tonnage of the Substance manufactured or imported in the EU is in the range of 100 – 1000 tonnes per year.

Furthermore, you reported that among other uses, the Substance is used as:
- Manufacture of 2,5-bis(1,1-dimethylpropyl) benzene-1,4-diol, including distribution, storing, handling and quality control
- Formulation of aqueous dispersions
- Use as antioxidant in medium/high voltage cross-linked polyethylene-sheathed (PE) cables
- Use as antioxidant in adhesives
- Use as stabilizer in uncured rubber
- Professional use as chemical for R&D
- Consumer use of adhesives
- Service life of articles from uncured rubber and adhesives (consumers).

Therefore, exposure to workers, consumers, and environment cannot be excluded.

1.3 Identification of the potential risk to be clarified

Based on all information available in the registration dossier and information from the published literature, the Substance, DAHQ, may be a PBT/vPvB substance due to potential PBT/vPvB properties of the relevant transformation product/impurity [redacted].

No experimental data are available for [redacted].

The information you provided on manufacture and uses demonstrates a potential for exposure of the environment.

Based on this hazard and exposure information, the Substance poses a potential risk to the environment.

As explained in Section 1.1 above, the available information is not sufficient to conclude on the hazard and on the P/vP/B/vB properties of the Substance. Consequently, further data is needed to clarify the potential risk related to PBT/vPvB properties of the Substance.

1.4 Testing strategy and further risk management measures

The current decision aims at clarifying the relevant physicochemical properties of the transformation product [redacted]. Based on this information, the evaluating MSCA will consider whether further testing and information to clarify P/vP and B/vB of [redacted] would be feasible and warranted to assess these properties for [redacted]. The further information will in turn allow to conclude on whether the Substance meets the criteria for PBT/vPvB substances.

If the PBT/vPvB properties(s) of the Substance are confirmed, the evaluating MSCA will analyse the options to manage the risk(s). New regulatory risk management measures could be identification as substance of very high concern and authorisation/restrictions of the use of the Substance for PBT properties.

2. How to clarify the potential risk

2.1 Vapour pressure (test method: EU A.4/OECD 104)

a) Aim of the study

The aim of the study is to obtain a vapour pressure value, which is relevant to clarify the volatility property of [redacted]

As it is expected that [redacted] volatility would hamper simulation testing and possible follow-up experiments, a proper understanding of its physicochemical property is critical to choose the most suitable approach for further testing on this transformation product.

In your comments on the draft decision, you agreed to perform the requested study.

b) Specification of the requested study

Test material

[redacted] with IUPAC name: [redacted].

Request for the full study report

You must submit the full study report which includes:

- a complete rationale of test design and
- interpretation of the results
- access to all information available in the full study report, such as implemented method, raw data collected, interpretations and calculations, consideration of uncertainties, argumentation, etc.

2.2 Determination of Henry's law constant (HLC)

a) Aims of the request

Volatilisation can be an extremely important removal process, with half-lives as low as

several hours.

The aims of the request are to clarify (i.) the environmental distribution behaviour and (ii.) the fate of [redacted].

The Henry's law constant (HLC) reflects the relative volatility of a particular substance and can give qualitative indications of the importance of volatilisation and is a key factor in determining the environmental fate of the substance by quantifying its partitioning between the aqueous and gas phases.

Information on HLC is also critical to choose the most suitable approach for further testing with this transformation product.

In your comments to the draft decision, you agreed that the information on HLC needs to be determined. However, you highlighted that HLC is not a common test to be conducted scientifically and is currently not available among the CROs that you have contacted. Therefore, you proposed that, if you cannot locate a laboratory to perform the test, you will determine the HLC via the calculation/estimation method and provide a list of laboratories contacted and an adequate justification for the calculation.

The ECHA Guidance acknowledges that the estimation of the HLC by the ratio of water solubility (c_w) and vapour pressure (vp) given at the same temperature (suitable for substances of low water solubility, i.e., < 1.0 mol/L) is not a highly accurate method, but neither is the measurement of HLC, especially for substances of very high or very low HLC values. As a result, while in the opinion of the evaluating MSCA, the experimental determination of the HLC remains the preferred way-forward to address the information request A.2., the draft decision has been amended so that the estimation of the HLC by the cw/vp ratio can also be accepted, provided that you are able to give evidence that no suitable testing laboratory could be located to conduct experimental measurements.

Therefore, you must determine the HLC according to one of the experimental approaches in Appendix R.7.1-1 of the ECHA Guidance[1]. The calculation/estimation method may be applied, if you are able to give evidence that no suitable testing laboratory could be located to conduct experimental measurements and submit an adequate justification for the calculation performed.

b) Specification of the request

Test material

[redacted] with IUPAC name: [redacted]

Request for the full study report if HLC is experimentally determined

You must submit the full study report which includes:

- a complete rationale of test design and
- interpretation of the results
- access to all information available in the full study report, such as implemented method, raw data collected, interpretations and calculations, consideration of uncertainties, argumentation, etc.

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2.3 Water solubility (test method: EU A.6/OECD TG 105)

a) Aim of the study

The water solubility of the Substance is very low (< 0.2 µg/L, measured according to the OECD TG 105).

The aim of the study is to determine the solubility of [redacted] in water, which is critical to choose the most suitable approach for further testing of this transformation product in environmental compartments. This is important to ensure that any ecotoxicity studies can be conducted using concentrations below the water solubility limit.

In your comments on the draft decision, you agreed to perform the requested study.

b) Specification of the requested study

Test material

[redacted] with IUPAC name: [redacted]

Request for the full study report

You must submit the full study report which includes:

- a complete rationale of test design and
- interpretation of the results
- access to all information available in the full study report, such as implemented method, raw data collected, interpretations and calculations, consideration of uncertainties, argumentation, etc.

2.4 Partition Coefficient 1-Octanol/Water (test method: Slow-Stirring Method, OECD TG 123)

a) Aim of the study

The estimation of log Kow from QSAR for [redacted] exceeds the threshold for B/vB screening.

The aim of the study is to assess the B property of [redacted]. The log K_{ow} is critical to choose the most suitable approach for further testing of this transformation product. Moreover, it can be useful as input to QSAR predictions.

In your comments on the draft decision, you agreed to perform the requested study.

b) Specification of the requested study

You must perform the test using the slow-stirring method, recommended for substances with an expected log K_{ow} >5, as it is considered the most appropriate and accurate method for hydrophobic substances.

Test material

[redacted] with IUPAC name: [redacted]

Request for the full study report

You must submit the full study report which includes:

- a complete rationale of test design and
- interpretation of the results
- access to all information available in the full study report, such as implemented method, raw data collected, interpretations and calculations, consideration of uncertainties, argumentation, etc.

Consideration of time needed to perform the requested study

In your comments to the draft decision, you sought to extend the deadline, based on the following justifications:

- You highlighted the current low capacity of Contract Research Organisations (CROs) due to current workloads and requested an extension of 9 – 12 months.

  ECHA notes that the deadline of the decision is set based on standard practice for performing OECD TG tests. However, ECHA has exceptionally extended the deadline by an additional 6 months, to take into account the current longer lead times in CROs.

- You highlighted that this substance is not commercially available and if a reputable supplier cannot be identified, a further extension of 12 months would be required to enable adequate sourcing and synthesis.

  ECHA and the evaluating MSCA consider that the substance is commercially available and therefore, in the absence of any documentary evidence to support your claims, ECHA considers that you have provided insufficient justification for an additional extension on this basis.

Consequently, ECHA has partially granted your request and extended the deadline from 6 months to 12 months.

Appendix C: Procedure

This decision does not imply that the information you submitted in your registration dossier(s) is in compliance with the REACH requirements. ECHA may still initiate a compliance check on your dossiers.

12-month evaluation

Due to initial grounds of concern for 2,5-di-tert-pentylhydroquinone (DAHQ), the Member State Committee agreed to include the Substance 2,5-di-tert-pentylhydroquinone (DAHQ) in the Community rolling action plan (CoRAP) to be evaluated in 2014. Italy was the competent authority ('the evaluating MSCA') appointed to conduct the evaluation in 2019.

In accordance with Article 46(1) of REACH, a substance evaluation decision was issued on 23 February 2016 requesting further information. You submitted information on 6 May 2021.

In accordance with Article 45(4) of REACH, the evaluating MSCA conducted its evaluation based on the information in the registration dossier(s) you submitted on the Substance and on other relevant and available information. The evaluating MSCA completed its evaluation considering that further information is required to clarify the following concerns: PBT/vPvB.

Therefore, it submitted a draft decision (Article 46(1) of REACH) to ECHA on 27 May 2022.

Decision-making

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

(i) Registrant(s)' commenting phase

ECHA received your comments and forwarded them to the evaluating MSCA.

The evaluating MSCA took your comments into account (see Appendix A). The request(s) and the deadline were amended.

(ii) Proposals for amendment by other MSCAs and ECHA and referral to the Member State Committee

The evaluating MSCA notified the draft decision to the competent authorities of the other Member States and ECHA for proposal(s) for amendment.

As no amendments were proposed, ECHA took the decision according to Articles 52(2) and 51(3) of REACH.

After the deadline set in this decision has passed, the evaluating MSCA will review the information you will have submitted and will evaluate whether further information is still needed to clarify the potential risk, according to Article 46(3) of REACH. Therefore, a subsequent evaluation of the Substance may still be initiated after the present substance evaluation is concluded.

Appendix D: Technical Guidance to follow when conducting new tests for REACH purposes

Test methods, GLP requirements and reporting

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.

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.

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[3].

Test material

1. *Selection of the Test material(s)*

   The Test Material used to generate the new data must be selected taking into account the impact of each constituent/ impurity on the test results for the endpoint to be assessed.

2. *Information on the Test Material needed in the updated dossier*

   a) 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.
   b) The reported composition must include all impurities and their concentration values.

Technical instructions on how to report the above is available in the manual "How to prepare registration and PPORD dossiers"[4].

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