EUROPEAN CHEMICALS AGENCY

Decision number: CCH-D-0000003056-80-09/F Helsinki, 14 February 2014

DECISION ON A COMPLIANCE CHECK OF A REGISTRATION PURSUANT TO ARTICLE 41(3) OF REGULATION (EC) NO 1907/2006

For Benzyl 3-isobutyryloxy-1-isopropyl-2,2-dimethylpropyl phthalate, CAS No 16883-83-3 (EC No 240-920-1), registration number [redacted]

Addressee: [redacted]

The European Chemicals Agency (ECHA) has taken the following decision in accordance with the procedure set out in Articles 50 and 51 of Regulation (EC) No 1907/2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH Regulation).

I. Procedure

Pursuant to Article 41(1) of the REACH Regulation ECHA has performed a compliance check of the registration dossier for Benzyl 3-isobutyryloxy-1-isopropyl-2,2-dimethylpropyl phthalate, CAS No 16883-83-3 (EC No 240-920-1) submitted by [redacted] (Registrant).

This decision is based on the registration dossier as submitted with submission number [redacted], for the tonnage band of 1000 tonnes or more per year. This decision does not take into account any updates after 5 September 2013, the date upon which ECHA notified its draft decision to the Competent Authorities of the Member States pursuant to Article 51(1) of the REACH Regulation.

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

The compliance check was initiated on 17 December 2012.

On 14 February 2013 ECHA sent the draft decision to the Registrant and invited him to provide comments within 30 days of the receipt of the draft decision.

By 18 March 2013 the Registrant did not provide any comments on the draft decision to ECHA.

On 5 september 2013 ECHA notified the Competent Authorities of the Member States of its draft decision and invited them pursuant to Article 51(1) of the REACH Regulation to submit proposals to amend the draft decision within 30 days of the receipt of the notification.

Subsequently, Competent Authorities of the Member States did not propose amendments to the draft decision and ECHA took the decision pursuant to Article 51(3) of the REACH Regulation.

II. Information required

Pursuant to Articles 41(1)(a), 41(3) and 10(a)(ii) as well as Annex VI , section 2 of the REACH Regulation the Registrant shall submit for the registered substance:

a. Composition of the substance (Annex VI, 2.3.), as specified under section III.(a) below;
b. Spectral data (Annex VI, 2.3.5), as specified under section III.(b) below;
c. Chromatogram (Annex VI, 2.3.6.) as specified under section III.(c) below;
d. Description of the analytical method or bibliographical references (Annex VI, 2.3.7.), as specified under section III.(d) below.

Pursuant to Article 41(4) of the REACH Regulation the Registrant shall submit the information in the form of an updated IUCLID dossier to ECHA by **14 May 2014.**

III. Statement of reasons

Based on the examination of the technical dossier, ECHA concludes that the information therein, submitted by the Registrant for registration of the above mentioned substance for the purpose of registration within the applicable tonnage band of 1000 tonnes or more per year in accordance with Article 6 of the REACH Regulation, does not comply with the requirements of Article 10 and with Annex VI thereof. Consequently, the Registrant is requested to submit the information mentioned above that is needed to bring the registration into compliance with the relevant information requirements.

Missing information related to substance identity

Pursuant to Article 10(a)(ii) and Annex VI, section 2 of the REACH Regulation, the technical dossier of the registration shall include information on the identity of the substance. Annex VI, section 2 lists information requirements that shall be sufficient to identify the registered substance.

(a) Composition of the substance (Annex VI, 2.3.)

The substance composition corresponds to the chemical representation of what the substance consists of and is therefore an essential part of substance identification and the cornerstone of all the REACH obligations.

ECHA notes that the registration does not contain sufficient and appropriate information for establishing the composition of the registered substance and therefore its identity, as required under Annex VI, section 2.3. of the REACH Regulation.

The Registrant identified the registered substance as a multi-constituent substance, however the compositional information included in IUCLID Section 1,2 indicate the presence of only one main constituent, namely "benzyl 3-(isobutyryloxy)-1-isopropyl-2,2-dimethylpropyl phthalate", with a purity level of [redacted] (w/w). ECHA underlines that the identification of the substance as a multi-constituent substance would indicate that both the R and S enantiomers of "benzyl 3-(isobutyryloxy)-1-isopropyl-2,2-dimethylpropyl phthalate" are the main constituents of the registered substance. However, the Registrant did not provide any information on the presence and the relative concentration level of these 2 enantiomers in IUCLID Section 1.2. of the dossier.

In addition, ECHA notes that the chromatographic analytical information (GC) reported in IUCLID Section 1.4 indicates the presence of 2 main peaks labelled "S278 1-TP-ISOMEER" and "S278 3-TP-ISOMEER". Neverthless, the identification of these two main peaks as well as their molecular and structural information were not reported.

Moreover, ECHA notes that in the gas chromatography-mass spectroscopy (GC-MS) analysis included in IUCLID Section 1.4, structural information was provided for 9 peaks identified in the gas-chromatogram. The two peaks labelled as "ETHYL-1-TP-PHTHALAAT" and "ETHYL-3-TP-PHTHALAAT" were identified as "benzyl 3-(isobutyryloxy)-1-isopropyl-2,2-dimethylpropyl phthalate" and "benzyl 3-(isobutyryloxy)-3-isopropyl-2,2-dimethylpropyl phthalate". In analogy with the name used for the identification of these two constituents, it can be inferred that the peaks labelled as "S278 1-TP-ISOMEER" and "S278 3-TP-ISOMEER" in the GC analysis do not designate enantiomers but regioisomers corresponding to "benzyl 3-(isobutyryloxy)-1-isopropyl-2,2-dimethylpropyl phthalate" and "benzyl 3-(isobutyryloxy)-3-isopropyl-2,2-dimethylpropyl phthalate". Each of these two regioisomers may be present in two different enantiomeric forms: R and S enantiomers.

ECHA therefore concludes that the identity and concentration level of the following stereo- and regio-isomers expected to be present in the composition of the registered substance is currently missing from the dossier:

- benzyl (1R)-3-(isobutyryloxy)-1-isopropyl-2,2-dimethylpropyl phthalate;
- benzyl (1S)-3-(isobutyryloxy)-1-isopropyl-2,2-dimethylpropyl phthalate;
- benzyl (3R)-3-(isobutyryloxy)-3-isopropyl-2,2-dimethylpropyl phthalate;
- benzyl (3S)-3-(isobutyryloxy)-3-isopropyl-2,2-dimethylpropyl phthalate.

The Registrant is accordingly requested to report the identity and concentration levels of each individual constituent present in the composition of the registered substance, including the four constituents listed hereinabove.

As for the reporting of the information in IUCLID, instructions on how to report the composition of well-defined multi-constituent substances are available in chapter 2.2.1.2. of the Data Submission Manual – Part 18: How to report the substance identity in IUCLID 5 for registration under REACH (version: 2.0, July 2012) on the ECHA website. The Registrant shall ensure in particular to distinguish between the main constituents (i.e. the constituents present at a concentration ≥ 10% and < 80%) and the impurities of the specific multi-constituent substance covered by this registration.

The Registrant is reminded that, in line with chapter 4.3 of the Guidance, the following applies to multi-constituent substances, including the registered substance:

- All main constituents shall be identified and reported individually; and
- All the impurities present at ≥ 1 % shall be identified and reported individually; and
- All the impurities relevant for the classification and/or PBT assessment shall be identified and reported individually.

For each constituent, including the main constituents and any impurity, the typical, minimum and maximum concentration level shall be specified. The Registrant shall comply with these requirements.

The Registrant shall also ensure that the identifiers specified in IUCLID section 1.1 of the registration dossier, including the chemical name, any other identifier and the molecular and structural information, designate the main constituents of the multi-constituent substance which is the subject of this registration. In particular, if the main constituents do not correspond or are not limited to "benzyl (1R)-3-(isobutyryloxy)-1-isopropyl-2,2-dimethylpropyl phthalate" and "benzyl (1S)-3-(isobutyryloxy)-1-isopropyl-2,2-dimethylpropyl phthalate", the Registrant shall replace the chemical name reported in the IUPAC name field of IUCLID section 1.1 by a chemical name that follows the generic format "Reaction mass of [IUPAC names of the main constituents]" and delete the CAS entry with CAS number 16883-83-3 currently specified in the dossier. In this situation, the Registrant shall however not remove or modify at this stage the EC entry with EC number 240-920-1 currently assigned to this registration for technical reasons, the registration being linked to that EC entry in REACH-IT. To ensure unambiguous identification of the registered substance, the Registrant shall instead specify, in the "Remarks" field of the reference substance in IUCLID section 1.1, the following: "The EC entry 240-920-1 currently assigned does not specifically correspond to the registered substance. This identifier can technically not be modified or deleted at this stage in the present registration update". The Registrant shall also specify, in the same IUCLID field, any available and appropriate EC number for the substance.

(b) Spectral data (Annex VI, 2.3.5.)

ECHA observes that the registration does not contain any appropriate NMR or mass spectra required according to Annex VI Section 2.3.5. of the REACH Regulation to support the identity of the registered substance.

ECHA notes that the Registrant attached a report from a gas chromatography-mass spectroscopy (GCMS) analysis of the registered substance to the dossier. The report includes a copy of a chromatogram and 9 mass spectra. However, ECHA can not relate the provided mass spectra to the recorded chromatogram. These spectra do not appear to be generated from the GCMS analysis of the registered substance but to originate instead from mass spectra libraries, as for instance in the case of the spectrum assigned to phthalic anhydride which refers to "mainlib". In addition, the mass spectra for all the constituents detected, including the main constituents eluting at ca. 20 min have not been included. ECHA therefore can not use the mass spectral data included in the registration to verify the identity of the constituents present in the composition of the registered substance.

The Registrant is therefore requested to submit appropriate NMR spectra (such as a ^{1}H and ^{13}C NMR spectra, including also, where relevant, the peak integrals) to support the identity of the constituents, including each main constituent, present in the composition of the registered substance. As an alternative or in complement to NMR spectra, mass spectra of the registered substance, including the main constituents, shall be provided to the extent they enable the resolution of the structure of these constituents.

As for the reporting of the spectral data in the registration dossier, the information shall be included in IUCLID section 1.4.

The Registrant shall ensure that the description of the analytical methods used for the recording of the spectra is specified in the dossier, in line with the requirements under Annex VI section 2.3.7.

(c) Chromatogram (Annex VI, 2.3.6.)

ECHA notes that copies of GC and High Performance Liquid Chromatography chromatograms have been attached to the dossier. However, ECHA observes that the Registrant did not provide any report from these chromatographic analyses. In particular, a peak table with the associated retention times and peak area has not been included. ECHA points out that this information is required since it constitutes a numerical representation of the chromatogram.

The Registrant is accordingly requested to provide the report from the chromatographic analyses of the registered substance.

As for the reporting in the registration dossier, the information shall be included in IUCLID section 1.4.

(d) Description of the analytical methods (Annex VI, section 2.3.7.)

ECHA observes that the Registrant did not provide any appropriate description of the analytical methods used for the identification and quantification of the constituents required to be reported in the composition of the registered substance, as requested according to Annex VI section 2.3.7.

More specifically ECHA notes that the Registrant provided results from a quantitative analytical method based on GC and HPLC chromatography and involving the use of internal standards. However, the protocol followed to record the chromatograms (including details of the sample preparation, the column specifications, identity of the carrier gas/eluents used, temperature/elution profile applied, identity of the internal standards) and complete details of the calculations made to derive the concentration of the constituents or groups of constituents present in the substance have not been included in the report. It follows that the results of these analyses can not be reproduced. In addition, the description of the analytical methods used for the identification and quantification of each of the 4 individual isomers expected to be present in the composition of the registered substance and quoted under point III.1.(a) of this decision is missing from the dossier.

The Registrant is accordingly requested to provide a description of the analytical methods used for the identification and quantification of the constituents and groups of constituents required to be reported in the composition of the registered substance. The description shall be sufficient for the methods to be reproduced and shall therefore include details of the experimental protocol followed, any calculation made and the results obtained.

As for the reporting of the data in the registration dossier, the information shall be attached in IUCLID section 1.4.

IV. Information on right to appeal

An appeal may be brought against this decision to the Board of Appeal of ECHA under Article 51(8) of the REACH Regulation. Such an appeal shall be lodged within three months of receiving notification of this decision. Further information on the appeal procedure can be found on ECHA's internet page at http://echa.europa.eu/appeals/app_procedure_en.asp. The notice of appeal will be deemed to be filed only when the appeal fee has been paid.

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