EUROPEAN CHEMICALS AGENCY

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

DECISION ON SUBSTANCE EVALUATION PURSUANT TO ARTICLE 46(1) OF REGULATION (EC) NO 1907/2006

For Isoheptane, CAS No 31394-54-4 (EC No 250-610-8)

Addressee: [redacted] registrant of isoheptane (concerned registrant)

Based on an evaluation by the Latvian Environment, Geology and Meteorology Centre (LEGMC) as the Competent Authority of Latvia (evaluating MCSA), the European Chemicals Agency (ECHA) has taken the following decision in accordance with the procedure set out in Articles 50 and 52 of Regulation (EC) No 1907/2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH Regulation).

This decision does not take into account any updates of the registration of the concerned registrant after 20 June 2013, the date upon which the draft decision was circulated to the other Competent Authorities of the Member States and ECHA pursuant to Article 52(1) of the REACH Regulation.

This decision does not imply that the information provided by the concerned registrant in the registration is in compliance with the REACH requirements. The decision neither prevents ECHA from initiating compliance checks on the dossier of the concerned registrant at a later stage, nor does it prevent a new substance evaluation process once the present substance evaluation has been completed.

I. Procedure

Pursuant to Article 45(4) of the REACH Regulation the Competent Authority of Latvia has initiated substance evaluation for Isoheptane, CAS No 31394-54-4 (EC No 250-610-8) based on a registration dossier submitted by the concerned registrant and prepared the present decision in accordance with Article 46(1) of the REACH Regulation.

On the basis of an opinion of the ECHA Member State Committee and due to initial grounds for concern relating to exposure to workers and possible PBT/vPvB properties, isoheptane was included in the Community rolling action plan (CoRAP) for substance evaluation pursuant to Article 44(2) of the REACH Regulation to be evaluated in 2012. The CoRAP was published on the ECHA website on 29 February 2012. The Competent Authority of Latvia was appointed to carry out the evaluation. During the course of evaluation the Competent Authority of Latvia noticed an issue related to the substance identity, which needs to be addressed in order to clarify the initial concern.

The Competent Authority of Latvia considered that further information was required to clarify the abovementioned concerns. Therefore, it prepared a draft decision pursuant to Article 46(1) of the REACH Regulation to request further information. It submitted the draft decision to ECHA on 28 February 2013.

On 20 March 2013 ECHA sent the draft decision to the concerned registrant(s) and invited them pursuant to Article 50(1) of the REACH Regulation to provide comments within 30 days of the receipt of the draft decision.

By 19 April 2013 ECHA received comments from concerned registrant(s) of which it informed the evaluating MSCA without delay.

The evaluating MSCA considered the comments received from the concerned registrant[s]. The information contained therein is reflected in the Statement of Reasons (Section III) whereas no amendments to the Information Required (Section II) were made.

In accordance with Article 52(1) of the REACH Regulation, on 20 June 2013 the evaluating MSCA notified the Competent Authorities of the other Member States and ECHA of its draft decision and invited them pursuant to Articles 52(2) and 51(2) of the REACH Regulation to submit proposals to amend the draft decision within 30 days.

Subsequently, ECHA submitted proposals for amendment to the draft decision.

On 26 July 2013 ECHA notified the concerned registrants of the proposals for amendment to the draft decision and invited them pursuant to Articles 52(2) and 51(5) of the REACH Regulation to provide comments on those proposals for amendment within 30 days of the receipt of the notification.

The evaluating MSCA has reviewed the proposals for amendment and did not amend the draft decision; however, the Statement of Reasons (Section III) of the draft decision was changed.

On 5 August 2013 ECHA referred the draft decision to the Member State Committee.

On 20 August 2013 the Registrant provided comments on the proposed amendments. The Member State Committee took the comments of the Registrant into account.

A unanimous agreement of the Member State Committee on the draft decision was reached on 9 September 2013 in a written procedure launched on 29 August 2013. ECHA took the decision pursuant to Article 51(6) of the REACH Regulation.

II. Information required

Pursuant to Article 46(1) of the REACH Regulation the concerned registrant shall submit the following information for the registered substance:

1) Name or other identifier of each substance,
2) Composition of the substance,
3) Spectral data,
4) Description of analytical methods or the appropriate bibliographical references for identification of the substance and, where appropriate, for the identification of impurities and additives.

Pursuant to Article 46(2) of REACH Regulation, the registrant shall submit the information in the form of an updated IUCLID dossier to ECHA by 20 March 2014.

III. Statement of reasons

Based on the evaluation of all relevant information submitted on isoheptane and other relevant and available information, ECHA concludes that further information is required in order to enable the evaluating MSCA to complete the evaluation of whether the substance constitutes a risk to human health or the environment.

During the course of the evaluation, the Competent Authority of Latvia identified substantial gaps and discrepancies with regard to the proper identification of the registered substance. After thorough analysis of the submitted analytical information, ECHA concluded that clarification on the substance identity is required in order to conclude on the potential PBT

properties of the registered substance, as initially indicated in the CoRAP. Thus, it is essential to define the exact identity of the registered substance before the weighing of the intrinsic properties of the constituents against the PBT criteria, as defined in the Annex XIII of the REACH Regulation (EC) No. 1907/2006, can be carried out. The same is a valid pre-condition for the proper evaluation of exposure aspects of particular constituents of the registered substance in the working environment. In addition, ECHA notices that identification of the substance in the isoheptane registration dossier represents also an information requirement, as outlined in Article 10 and Annex VI of the REACH Regulation (EC) No. 1907/2006.

1) Name or other identifier of each substance

Based on the examination of the registration data from the technical dossier, ECHA notices that the Registrant uses very generic identifiers in description of the substance identity. The name provided for the substance, its EINECS and CAS numbers, as well as INChI and SMILES formulas refer to a mixture of [redacted] different isomers. However, gas chromatography (GC) data provided in the registration dossier shows that none of the constituents in the registered substance is present in concentration of at least 80% (w/w). GC distinguishes following substances in the concentration range between [redacted]. In accordance with submitted GC few other substances are present in the registered substance in the concentration range between [redacted], i.e. [redacted].

In line with the Guidance for identification and naming of substances under REACH and CLP[1], mono-constituent substance is a substance, defined by its quantitative composition, in which one main constituent is present to at least 80% (w/w); consequently, based on the information available in the dossier the registered substance would be considered a multi-constituent substance.

ECHA also observes that the Registrant did not provide appropriate information on the name of the substance, as required under Annex VI Sections 2.1 and 2.2 of the REACH Regulation.

Furthermore, Article 10(a)(ii) and Annex VI, sections 2.1 and 2.2 of the REACH Regulation requires that the technical dossier of the registration includes information on the identity of the substance that shall be sufficient to identify the registered substance.

In his comments to the proposal for amendments submitted by ECHA, the Registrant committed to updating his dossier with information showing that the substance meets the definition of a UVCB substance.

Therefore, the Registrant is requested to remove generic descriptors (name, EC number, CAS number) of the registered substance, and to adjust information in the Registration Dossier, clearly and explicitly demonstrating in the Section 1.2 of the IUCLID dossier the nature of the registered substance,

a) Naming the substance is accordance with Guidance for identification and naming of substances under REACH and CLP Chapter 4.2.2,

b) Providing EINECS or ELINCS number (if available and appropriate) for every main constituent of the substance,
c) Providing CAS name and CAS number (if available) for every main constituent of the substance,
d) Providing other identity code (if available) for every main constituent of the

[1] http://echa.europa.eu/web/guest/guidance-documents/guidance-on-the-different-methods-under-reach

substance

2) Composition of the substance

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 corner stone of all the REACH obligations.

ECHA notes that the registration does not contain sufficient 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.

More specifically, ECHA notes that the Registrant identified the registered substance as a mono-constituent substance. In line with the Guidance for identification and naming of substances under REACH and CLP, mono-constituent substance is a substance, defined by its quantitative composition, in which one main constituent is present to at least 80% (w/w). However, the registration dossier, when identifying a substance, contains description of generic identifiers for the registered substance (EINECS number, CAS number, and IUPAC name) that refers to the mixture of [redacted] different isomers of the substance.

Additionally, ECHA notes that the substance composition in the chromatogram is different from the one in the Section 1.2 of the technical dossier – certain impurities are not mentioned at all, while few, present in lower concentration than 1% (w/w) are named as being impurities.

Regarding how to report the composition of the registered substance in IUCLID, the following applies: The Registrant shall report individually any constituent and impurity required to be identified and specify at least one of the following identifiers: chemical name, CAS number, EC number and/or molecular formula, as well as the minimum, maximum and typical concentration, in the appropriate fields in Section 1.2 of the IUCLID dossier. The Registrant shall also provide accurate information on the degree of purity of the registered substance and/or the concentration range of the main constituent and any impurity reported in Section 1.2 of the IUCLID dossier to ensure that the information provided is consistent. The Registrant shall ensure that the information provided on the composition of the substance is confirmed by the analytical data included in section 1.4 of the IUCLID dossier.

Further technical details on how to report the composition of multi-constituent substances in IUCLID are available in paragraphs 2.1 and 2.2.1.2. of the Data Submission Manual 18 on the ECHA website at:
http://echa.europa.eu/doc/reachit/dsm18/substance_id_report_iuclid_en.pdf.

3) Spectral data

ECHA notes that the registration dossier contains neither infra-red (IR) nor nuclear magnetic resonance (NMR) spectral data which are required according to Annex VI, Section 2.3.5 of the REACH Regulation to support the indicated substance identity. Instead, the Registrant includes justifications for not providing this information. According to the justifications, the Registrant considers the required spectral data as scientifically unnecessary to identify the substance.

Contrary to the Registrant, ECHA regards the required spectral data as scientifically necessary for the identification of the registered substance for the following reasons:

- The IR spectrum displays characteristic vibration bands of the molecules present in the substance. Although no functional groups might be present in the molecules of the registered substance, alkanes have characteristic vibration bands which can be recorded

in the spectrum. As a consequence, the IR spectrum provides information of the identity of the substance; and

- An NMR spectrum, such as a ^{1}H-NMR, is relevant tool for molecular structure characterization of well-defined organic substances due to characteristic chemical shifts and spin-spin coupling, which also reflect the relative abundance of individual atoms.

Moreover, ECHA points out that IR and NMR spectral data are standard requirements of Annex VI, Section 2.3.5.

Therefore, the Registrant is requested to submit an IR spectrum and an NMR spectrum, such as a ^{1}H-NMR. As an alternative to the NMR spectrum, a mass spectrum (MS) of the registered substance can be provided.

As for the reporting of the spectral data in the registration dossier, the spectra should be attached in IUCLID section 1.4.

4) Description of analytical methods or the appropriate bibliographical references for identification of the substance and, where appropriate, for the identification of impurities and additives

ECHA observes that the registration does not contain sufficient details of the analytical methods to identify the registered substance, including its composition.

The Registrant provides only the result of gas chromatogram analysis including the peak list and chromatogram.

Whilst this method can be used for the quantification of the main constituents and impurities, the registrant did not include sufficient details for such method to be regarded as a quantitative analysis that can be reproduced. In particular, ECHA notes that the report does not include detailed information on the experimental parameters used for the recording of the chromatogram (such as the column temperature program, injector temperature, detector temperature, detector gas supply flow, carrier gas flow).

Accordingly, in correspondence with Annex VI, 2.3.7 of the REACH Regulation, the Registrant is requested to submit the description of the missing analytical methods, or the appropriate bibliographical references, to identify the registered substance, including its composition. The information shall be sufficient for each method to be reproduced and shall therefore include details of the experimental protocol followed, the calculation used and the result obtained.

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

In his comments, the Registrant clarified that considering the substance at issue a UVCB substance would be most appropriate. The Registrant furthermore confirmed his strong commitment to updating the registration dossier within three months of the decision and provide specific and detailed substance identity information in order to meet the concerns that ECHA raised in this decision.

Following the receipt of the information outlined in Section II of the draft decision, the Competent Authority of Latvia will be able to address the concerns indicated in the CoRAP.

IV. Information on right to appeal

An appeal may be brought against this decision to the Board of Appeal of ECHA under

Articles 52(2) and 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 the 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.

[redacted]

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