Helsinki, 26 November 2021

Addressees
Registrants of Alkanes, C16–(branched), C20-(branched) and C24-(branched) listed in the last Appendix of this decision

Registered substance subject to this decision ('the Substance')
Substance name[1]: Alkanes, C16–(branched), C20-(branched) and C24-(branched)
List number: 700-992-1

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 using the **isomer 3,4,5,6,7,8-hexamethyldecane**, a structure likely to be present in the UVCB, as test substance:

Environment

1. Simulation testing on ultimate degradation in surface water (test method: Aerobic mineralisation in surface water – a modified version of the simulation biodegradation test, EU C.25/OECD TG 309) under the following test conditions:

- perform the pelagic test – without additional suspended solids/sediment, containing a natural concentration of ~15 mg SPM dw/l;
- at a test temperature of 12 °C;
- use sealed vessels with minimized headspace (to account for the combination of high air/water partitioning coefficient and low water solubility);
- the test material must have the highest purity possible, documented by GC and NMR analysis;
- use a ^{14}C radiolabelled test substance (to appropriately verify the degradation kinetics and mass balance); you must provide justification for the location of the radiolabel on the test substance, which must be in the most stable part of the molecule;
- take into account the initial loss of substance from the water phase to air (to calculate a mass balance);
- include sterile controls and a justification of the method and procedure used for establishing the sterile controls;
- measure the concentration of the test substance at appropriate intervals during the study so that a reliable primary degradation half-life can be determined;
- transformation and/or degradation products must be identified and quantified at a concentration of ≥ 10% w/w. Transformation and/or degradation products of which concentrations are continuously increasing must also be considered;
- a mass balance must also be provided;
- quantify the total amount of non-extractable residues (NER) and the reporting of results must include a scientific justification of the used extraction procedures and solvents.

[1] previously registered as Alkanes, C16-20-iso, EC No 292-461-1, CAS RN 90622-59-6

If it can be demonstrated by sound justification that simulation testing in surface water is not technically feasible (*i.e.*: impossible to analytically quantify the parent compound), the following test is required instead:

Simulation testing on degradation in sediment (test method: Aerobic and anaerobic transformation in aquatic sediment systems – a modified version of the simulation biodegradation test, EU C.24/ OECD TG 308), under the following test conditions:

- at a test temperature of 12 °C;
- under aerobic conditions;
- include sterile controls and a justification for the method and procedure used to establish the sterile controls;
- the test material must have the highest purity possible, documented by GC and NMR analysis;
- use a concentration appropriate to also successfully identify and quantify possibly formed transformation and/or degradation products;
- transformation and/or degradation products must be identified and quantified at a concentration of ≥ 10% w/w. Transformation and/or degradation products of which concentrations are continuously increasing must also be considered;
- use a ^{14}C radiolabelled test substance (to appropriately verify the degradation kinetics and mass balance); you must provide justification for the location of the radiolabel on the test substance, which must be in the most stable part of the molecule;
- a mass balance must also be provided;
- quantify the total amount of non-extractable residues (NER) and the reporting of results must include a scientific justification of the used extraction procedures and solvents.

Deadline

The information required must be generated and submitted by **04 December 2023** from the date of the decision.

Conditions to comply with the information requested

To comply with this decision, you must provide the information in an update of the registration dossier(s), by the deadline indicated above, including robust study summaries and, where relevant, an update of the chemical safety report. Section B.1 of Appendix 1 provides further details on how the deadline was derived.

In addition to the robust study summaries, you must submit the full study report for the simulation testing on ultimate degradation by the same deadline, by attaching it to the relevant endpoint study record in IUCLID.

Appendices

The reasons of this decision and any further test specifications of the requirements are set out in Appendix 1. The procedural history is described in Appendix 2. Further information, observations and technical guidance as appropriate are provided in Appendix 3. Appendix 4 is an excerpt from the first decision for the Substance in 2016 (ECHA, 2016a), with additional information on modelling and comparable substances. Appendix 5 contains a list of registration numbers for the addressees of this decision. This appendix is confidential and not included in the public version of this decision.

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 Christel Schilliger-Musset, 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 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 1: Reasons to request information to clarify the potential risk

Based on the evaluation of all relevant information submitted on Alkanes, C16–(branched), C20-(branched) and C24-(branched) (hereinafter "the Substance"), and other relevant available information, ECHA concludes that further information is required to enable the evaluating Member State competent authority (MSCA) to complete the evaluation of whether the Substance constitutes a risk to the environment. 3,4,5,6,7,8-hexamethyldecane is an isomer that is likely to be present in the Substance and is considered as a reasonable worst case structure regarding the possible P-properties for the C16 fraction of the Substance.

A.1 The potential risk – environment

The identification of a potential risk is based on a combination of exposure and hazard information.

According to information in the registration dossier the Substance is used as a [redacted] in plastisols, in paper manufacturing, as a waste water treatment chemical, as a laboratory chemical, as a hydraulic fluid/lubricant in general manufacturing of machinery, in metal and offshore industry and is used in fuels and cosmetic products. Significant exposure to the environment cannot be excluded.

Based on information in the registration dossier as detailed below, there is a concern that the Substance may be a PBT or vPvB substance as defined in Annex XIII of REACH due to the properties of some isomers. Annex XIII provides that the identification of PBT/vPvB substances must also take account of the PBT/vPvB properties of relevant isomers of a substance.

Based on this exposure and hazard information, there is a potential risk for the environment. As the available information is not sufficient to conclude on potential PBT/vPvB properties, further information is needed.

A.2 The possible risk management measures – environment

If the obtained data from the request above, and subsequent studies to elucidate B and T properties, show that the Substance or relevant transformation and/or degradation products has PBT/vPvB properties as defined in Annex XIII of REACH, the evaluating MSCA will assess the need for further regulatory risk management in the form of identification as a substance of very high concern (SVHC) under Article 57 of REACH and subsequent authorisation or restriction of the Substance.

As the Substance is currently not regulated, this would lead to stricter risk management measures, such as minimisation of releases.

A.3 Explanation of the testing strategy – environment

In a first step, an enhanced OECD TG 310 test was requested in a decision in 2016 (ECHA, 2016a). Through modelling done by the evaluating MSCA (eMSCA) it was shown that the most branched isomers (with 4, 5 and 6 branches) in the C16 fraction are the ones that are most likely to be persistent and bioaccumulative, as shown in Appendix 4, table 1.

A more elaborate strategy than the one outlined in OECD TG 310 was needed to describe the degradation of the most branched isomers in the C16 fraction.

The results of the OECD TG 310 test did not show that the Substance as a whole was readily biodegradable. Further, the test confirmed that the least biodegradable C16-isomers are the most branched ones (as represented by the 3 first peaks of the C16 in the GC attached to the registration dossier). Therefore, in a second step of the testing strategy, a simulation test is needed (current request) to clarify the concerns for PBT/vPvB of the Substance.

Due to technical difficulties to test the Subtance as such, it was decided to request that the study be performed on a selected representative structure. This representative structure is based on the production process of the Substance and is considered to be the most branched C16-isomer that can be manufactured in the production process. The isomer is also likely to be a part of the Substance, but since the Substance is a UVCB and has a variable composition, this is not possible to verify for every batch produced.

This structure is representative of the isomers in the Substance that have the greatest potential to have both P and B properties, based on modelling performed by the eMSCA (Appendix 4, table 2). After careful consideration and discussions with you, the following structure is considered to represent the "reasonable worst case" regarding possible P-properties for the C16 fraction:

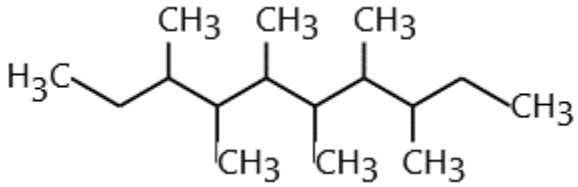

Fig 1 – Representative structure 3,4,5,6,7,8-hexamethyldecane

Therefore the request aims to clarify whether 3,4,5,6,7,8-hexamethyldecane, an isomer likely present in the Substance, may be characterised as persistent or very persistent. If the results of the required biodegradation test show that 3,4,5,6,7,8-hexamethyldecane is persistent or very persistent or any relevant transformation and/or degradation products has PBT/vPvB properties as defined in Annex XIII of REACH, the Substance will also be considered as persistent or very persistent.

This will further necessitate characterisation of bioaccumulation and possible toxicity of the Substance in a later tier.

There is currently not enough information available to justify a concern for toxicity. However, you have recently updated your registration dossier with new toxicity studies on an analogue substance (Repeated dose toxicity and prenatal developmental toxicity in the first species). Further studies (prenatal developmental toxicity on the second species and extended one generation toxicity) on the same analogue substance are reportedly on-going.

The eMSCA has not evaluated these new studies, but they could potentially reveal a concern for T. Therefore, for the time being the eMSCA will not disregard a T-concern and thus considers both P and B, as well as vP and vB properties.

A.4 The concern identified and why new information is needed

Your assessment concludes that the Substance is not PBT. However, the eMSCA has concerns that certain isomers in the Substance possibly have PBT/vPvB properties.

According to ECHA Guidance (IR&CSA, R.11, June 2017) on PBT/ vPvB assessment[3], Section R.11.4.1, a constituent (*i.e.* isomer in the Substance) should normally be considered relevant for the PBT/vPvB assessment when present at a concentration of ≥ 0.1% (w/w).

Based on the ^{13}C-NMR spectrum of the Substance in the registration, the eMSCA considers that, since the Substance has an average branching of 3, it will contain a considerable amount of isomers with 4, 5 and 6 branches, well above 0,1% (w/w), which may have PBT/vPvB properties according to eMSCA modelling (see Appendix 4, table 1). The biodegradation study (OECD TG 310) also indicated that a considerable portion of the Substance will not readily degrade, and that the isomers that are least likely to be readily degraded are the ones that are more highly branched. The representative structure of the Substance therefore needs to be evaluated for P properties.

a) Branching degree of the Substance and modelling performed by the eMSCA

The Substance is poorly water-soluble and has a complex and variable composition. It is made through [redacted] for petroleum substances), to yield a product with discrete carbon numbers: C16, C20 and C24 as well as highboilers.

The gas chromatograms (GC) in the registration dossier demonstrate that there are many C16-, C20- and C24-isomers present in the tested sample, but it is not possible to determine which ones from the supplied information (document accompanying the registration [redacted]. Thus, although the Substance is identified with a single List number, it contains many different isomers with an unknown degree of branching.

Branching degree affects many important properties of branched alkanes, *e.g.* the Substance, such as the boiling point and the vapour pressure in addition to the biodegradation and bioaccumulation. Based on NMR spectra in the registration dossier, the average branching is close to 3, and the substance consists of isomers with varying degrees of branching. You have not considered this in the CSR and no detail is available about the actual branching of each carbon fraction (*i.e.* C16, C20 and C24).

Comparison to screening tests from other hydrocarbons with comparable carbon number and registrant-performed read-across[4] shows that the criterion for ready biodegradation was achieved in some cases, while in other cases the substances were considered not readily biodegradable. The substances that contain isomers with more branching or cyclic substructures degrade to a lesser extent than linear and less branched ones. Determining the biodegradation potential of UVCBs can be challenging, as ready biodegradation test systems and study designs are not capable of distinguishing the relative contribution of the substances' isomers to the total biodegradation measured and the UVCB itself may still contain a certain amount of persistent isomers.

It is not feasible (nor justifiable) to determine the PBT/vPvB properties of every isomer based on experimental information.

[3] https://echa.europa.eu/documents/10162/13632/information_requirements_r11_en.pdf

[4] Alkanes, C12-26-branched and linear, EC number: 292-454-3
Hydrocarbons, C14-C20 n-alkanes <2 % aromatics, EC number: 923-583-1
Hydrocarbons, C16-C20 n-alkanes, isoalkanes, cyclics, <2 % aromatics, EC number: 919-029-3
C8-C26 branched and linear hydrocarbons – Distillates, EC number: 481-740-5
Distillates (Fischer-Tropsch), heavy, C18-50 - branched, cyclic and linear, EC number: 482-220-0

Based on the information on the manufacturing process in your registration dossier, the eMSCA therefore drew up representative structures and used modelling to estimate the persistence and bioaccumulation properties for different isomers in the Substance. These indicated that C16 isomers with 4 branches or more may constitute a P/vP and B/vB concern as they are potentially persistent and bioaccumulative.

For more information on the modelling performed and comparable substances see appendix 4, additional information.

Based on the modelling it was concluded that the C16 isomers with 4 branches or more could constitute a P/vP and B/vB concern.

b) Ready biodegradation studies in the dossier

In the registration dossier, two ready biodegradation studies are available.

- *ISO Draft 10708 (BOD Test for Insoluble Substances from 1993) for testing ultimate aerobic degradability of poorly soluble chemicals.*

In this study the Substance was tested above its water solubility and adsorption could therefore not be excluded. Activated sludge from a domestic sewage treatment plant was used as inoculum. The results of the test showed a biodegradation value of 32.2 % based on oxygen consumption after 28 days. In order to be called readily biodegradable, the test substance must show 60% degradation within the 10-day window. Therefore the Substance as a whole is not readily biodegradable and is therefore considered to be potentially P or vP.

To fulfil the PBT/vPvB criteria according to Section 1.1.1 of Annex XIII to REACH, the half-life cut-off value is of 40 days in freshwater. You calculated a half-life value of the Substance to be 47.5 days. However, it is not justifiable to calculate the half-life by extrapolating from a ready biodegradability test because such studies are screening tests and are not designed to measure the degradation half-life. Ready biodegradability tests are stringent tests which use a high concentration of the test substance. Their aim is not to predict degradation in the 'real world', but to screen whether a substance can be expected to degrade rapidly and completely (OECD, 2006). Therefore a conclusion on the fulfilment of the Annex XIII criteria cannot be reached using these studies.

- *New ready biodegradability study, requested by the first decision (ECHA, 2016a)*

As a result of the first tier of the substance evaluation of the Substance, an information request for a new ready biodegradability test (OECD TG 310 test) on the Substance was made.
Biodegradation was tested using method OECD TG 310 (Ready Biodegradability - CO2 in Sealed Vessels (Headspace Test)) with GC characterisation of the Substance before and after the test. Activated sludge from a domestic sewage treatment plant was used as inoculum. The rate of biodegradation was determined by measurement of the total inorganic carbon (TIC). The complex mixture of isomers in the C16-fraction of the Substance was divided into three groups according to presumed length of their carbon backbone and number of methyl groups. This gave an indication of their degree of branching, using an increment system, as described by Kovats (1958). The study was well performed, and provided further confirmation that the Substance as a whole was not readily biodegradable.
The group with most branching ("Group 1"), was not readily biodegradable. "Group 1" is assessed to constitute at least 10% of the Substance. If the isomers included in this group

are found to be P/vP, this would therefore be enough to characterise the whole Substance as P/vP. The isomers in Group 1, are also the ones that are most likely to be B/vB.

Results of the QSAR estimates and ready biodegradability screening tests show that several isomers in the C16 fraction could be P or vP. No simulation test on the degradation half-life of the C16 fraction of the Substance in soil, water or sediment is available. Therefore, it cannot be concluded whether the isomers in the C16 fraction meet the P criteria set out in Annex XIII of REACH. A simulation test, with adjustments to specifically study 3,4,5,6,7,8-hexamethyldecane, as a respresentative structure of the most branched C16 isomers, is therefore needed to clarify the concern of persistency in a tiered approach.

A.5 Considerations on the test method

a) Test material

The aim of the study is to determine the half-life of 3,4,5,6,7,8-hexamethyldecane. The test material must have as high a purity as possible, documented by GC and NMR analysis.

In your comments to the proposals for amendments, you state that the purity specifications should only be a recommendation and not mandatory. The specific purity of the substance is not a fixed number, but we consider it is important, and thus mandatory, that the highest purity that is possible to achieve is documented by GC and NMR analysis.

b) Test method

There are three types of simulation tests, OECD TG 307, 308 and 309. The OECD TG 309 is the preferred choice for testing of 3,4,5,6,7,8-hexamethyldecane for the following reasons:

- The ECHA Guidance (IR&CSA, R.11) on PBT/vPvB assessment (ECHA, 2017), states that when deciding on the relevant test compartment(s) for simulation testing, it is recommended to start testing with the OECD TG 309 if it is technically feasible.
- Information from the OECD TG 309 can be directly compared to the P-criterion for the aquatic aerobic compartment in the PBT assessment, if the test is performed in a way that reflects the environmental conditions of the aquatic aerobic compartment sufficiently well.
- 3,4,5,6,7,8-hexamethyldecane may be expected to form NERs. This assumption is based on the estimated Log K_{OC} of 3,4,5,6,7,8-hexamethyldecane (6.73)[5]. The NER formation in the OECD TG 309 is low, which will minimize any potential interpretation problems related to the NER formation.

In the OECD TG 309, two test options are described: the "pelagic test" and the "suspended sediment test". ECHA considers that the "pelagic test" option must be followed as that is the recommended option for P assessment. However, if it can be demonstrated by sound justification that simulation testing in surface water (OECD TG 309) is not technically feasible (*i.e.*: impossible to analytically quantify the parent compound), then an OECD TG 308 sediment simulation test must be performed instead.

ECHA suggests that you study the water solubility of the test substance using the OECD TG 123 slow stirring method. This is not a mandatory study but will give valuable information for choosing the best simulation test and for the further testing strategy of the Substance for bioaccumulation, if it is demonstrated to be P or vP.

[5] Estimated by the KOCWIN Program (v2.00) in OECD QSAR toolbox.

A review on determining the water solubility of difficult-to-test substances (Birch et al. 2019) is available and may be useful. It is stated in the OECD TG 308 that for the determination of biodegradation kinetics, the concentrations of the test substance must be below its water solubility. It should be noted that literature values of water solubility may differ from the solubility of the test substance in natural waters. Therefore, it may be useful to establish the solubility of the test substance by use of the natural waters being tested in the simulation tests.

The aim of the request is to test 3,4,5,6,7,8-hexamethyldecane as the representative structure of the C16-fraction of the Substance in an environmentally relevant test system with a small surface area for adsorption. The test system must be set up to ensure that NER-formation is kept to a minimum. The amount of suspended solids in the pelagic test should be representative of the level of suspended solids in EU surface water. The concentration of suspended solids in the surface water sample used must therefore be approximately 15 mg dw/l. Natural surface water containing between 10 and 20 mg SPM dw/l is considered acceptable.

In your comments to the proposals for amendments you outlined your intended approach to design the study according to OECD TG 309, namely:

- Synthesis of radiolabelled and non-radiolabelled test substance.
- Performance of preliminary tests on non-radiolabelled test substance to investigate the physical-chemical properties of the substance.
- Development of an analytical detection method
- Performance of pre-tests to determine an appropriate study design and feasibility of a closed study set-up, with potential inclusion of a sterile control with comparable test conditions.
- Decision on the feasibility of performing an OECD TG 309 test, or whether alternative test methods (OECD TG 308) is more appropriate.
- Generation of a study plan detailing the final study design and justification for selection of the appropriate test method.

Furthermore, you expressed again the wish to have a dialogue with the eMSCA at appropriate times to discuss and come to agreement on the design of a reliable study. ECHA notes that communication with the eMSCA is possible after the final decision has been issued to clarify any additional uncertainties regarding performing of the test.

c) <u>Test method adaptations for OECD TG 309</u>

- *Adaptations to address the volatility of the Substance*

You have submitted data on the vapour pressure for the whole Substance (< 1 hPa at 20°C), indicating a low volatility. However, this is not a reliable value as the expected low volatility of the higher weight C20- and C24-isomers may mask the volatility of the C16-isomers. The measured Henry's law constant for linear C16 is reported as 0,47 atm·m^3/mol, and all C16-isomers in the Substance are expected to be equally or slightly more volatile.

The volatility of the the test substance will therefore likely be too high for the standard OECD TG 307, 308 and 309 tests, and adaptation of the test is therefore necessary:

- Sealed vessels with a minimized headspace to account for the combination of high air/water partitioning coefficient and low water solubility of the test substance. Redox conditions in the test vessel must also be monitored throughout the test.

- The initial loss of substance from solution to air must be accounted for in order to assess the mass balance of the substance in the test system.
- Sterile controls must be performed and a justification of the method and procedure used for establishing the sterile controls must be provided. The inclusion of sterile controls is important to determine to what extent the decrease of the test substance is due to potential contribution of abiotic losses.

- *Measurement of test substance concentration and primary degradation*

The concentration of the test substance must be measured at appropriate intervals during the study so that a primary degradation half-life can be determined. This is required for the following reasons:

- The measurement of the test substance concentration is important for the comparison between the active test and sterile controls, to estimate the potential contribution of abiotic losses to the decrease in test substance concentration.
- Primary degradation half-life of the test substance is important for the conclusion on the P/vP property in case that degradation half-life based on residual ^{14}C is above the P or vP criterion and must be determined (in parallel with the determination of a half-life based on residual ^{14}C activity or the evolved $^{14}CO2$).
- Primary degradation half-life of the test substance may be important for the estimation of the persistence of any relevant transformation and/or degradation products.

- *Measurement of transformation and/or degradation products*

Transformation and/or degradation products detected at ≥10% of the applied concentration of the test substance at any sampling time must be identified unless reasonably justified otherwise, as they may be relevant for PBT/vPvB assessment. Transformation and/or degradation products of which concentrations are continuously increasing or seem to be stable during the study must also be considered for identification, even if their concentrations do not exceed the limit given above, as this may indicate persistence.

- *Test temperature*

Paragraph 24 of the OECD TG 309 specifies that the test should be performed at a controlled temperature ±2°C. The temperature may be the field temperature or a standard temperature of 20 to 25°C according to the TG. According to ECHA Guidance R7b, Section R.7.9.4.1, studies to determine whether a substance is persistent or very persistent are normally carried out at a temperature of 12°C because this is considered to be the average temperature of waters in Europe throughout the year. ECHA has selected a test temperature of 12°C as appropriate for identification for determination of the degradation half-life in this case. Therefore, the study must be conducted at 12°C.

- *Recovery and radiolabelling*

The total recovery should be in accordance with OECD TG 309, paragraph 52. The test substance must be radiolabelled due to its low water solubility for an appropriate verification of the degradation kinetics and mass balance. You must provide justification for the location of the radiolabel on the molecule.

- *Quantification of the total amount of non-extractable residues (NER)*

As specified in ECHA Guidance R.7.9.4.1., the organic carbon (OC) concentration in surface water simulation tests is typically 2 to 3 orders of magnitude higher than the test substance concentration and the formation of NERs may be significant in surface water tests.

- You must explain and scientifically justify the extraction procedure and solvent used obtaining a quantitative measure of NERs.
- The total amount of NER must be quantified, to demonstrate that all transformation and/or degradation products which have formed have been extracted and can be quantified. By default, total NER is regarded as non-degraded parent. 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 R.11.4.1.1.3.).
- You have the option to further characterise the types of NER to refine the P assessment. The Background note on 'Options to address NER in regulatory P assessment', published on the ECHA website provides some suggestions on the further refinement (https://echa.europa.eu/documents/10162/13632/bg_note_addressing_non-extractable_residues.pdf/e88d4fc6-a125-efb4-8278-d58b31a5d342).

d) Test method adaptations for OECD TG 308, if the OECD TG 309 cannot technically be performe

- *Adaptations to address the volatility of the Substance*

You have submitted data on the vapour pressure for the whole Substance (< 1 hPa at 20°C), indicating a low volatility. However, this is not a reliable value as the expected low volatility of the higher weight C20- and C24-isomers may mask the volatility of the C16-isomers. The measured Henry's law constant for linear C16 is reported as 0,47 atm·m^3/mol, and all C16-isomers in the Substance are expected to be equally or slightly more volatile.

The volatility of the the test substance will therefore be too high for the standard OECD TG 307, 308 and 309 tests, and adaptation of the test is therefore necessary:

- The mass balance of the substance in the test system must be provided.

It may be necessary to use sealed vessels with a minimized headspace to account for the combination of high air/water partitioning coefficient and low water solubility of the test substance.

- *Measurement of test substance concentration and primary degradation*

As described in the OECD TG 308, concentration of the test substance must be measured at appropriate intervals during the study so that a primary degradation half-life can be determined. This is required for the following reasons:

- Primary degradation half-life of the test substance is important for the conclusion on the P/vP property.
- Primary degradation half-life of the test substance may be important for the estimation of the persistence of the transformation products.

- *Measurement of transformation and/or degradation products*

Transformation and/or degradation products detected at ≥10% of the applied concentration of the test substance must be identified and quantified at every sampling time unless reasonably justified otherwise, as they may be relevant for PBT/vPvB assessment. Transformation and/or degradation products of which concentrations are continuously increasing or seem to be stable during the study must also be considered for identification, even if their concentrations do not exceed the limit given above, as this may indicate persistence.

An MSCA submitted a proposal for amendment, to include a request to perform an OECD TG 308 test, which included the identification/quantification of transformation and/or degradation products at a concentration of ≥ 1% w/w. The evaluating MSCA considered that in this specific case there was insufficient justification to deviate from the REACH guidance (R.11), which states that 'in general transformation products detected at ≥ 10% of the applied radioactivity in the total water-sediment system at any sampling time should be identified unless reasonably justified otherwise'. Consequently, a conditional request to perform an OECD TG 308 test was included in the decision, which includes identification/quantification of transformation and/or degradation products at a concentration of ≥ 10% w/w.

- *Test temperature*

Paragraph 33 of the OECD TG 308 specifies that the test should be "performed in the dark at a constant temperature in the range of 10 to 30 °C. A temperature of (20±2) °C is appropriate. Where appropriate, an additional lower temperature (e.g. 10 °C) may be considered on a case-by-case basis, depending on the information required from the test. Incubation temperature should be monitored and reported". According to ECHA Guidance R7b, Section R.7.9.4.1, studies to determine whether a substance is persistent or very persistent are normally carried out at a temperature of 12°C because this is considered to be the average temperature of waters in Europe throughout the year. ECHA has selected a test temperature of 12°C as appropriate for identification for determination of the degradation half-life in this case. Therefore, the study must be conducted at 12°C.

- *Recovery and radiolabelling*

The total recovery should be in accordance with OECD TG 308, paragraph 13. The test substance must be radiolabelled due to its low water solubility for an appropriate verification of the degradation kinetics and mass balance. You must provide justification for the location of the radiolabel on the molecule.

- *Quantification of the total amount of non-extractable residues (NERs)*

As specified in ECHA Guidance R.7.9.4.1., the organic carbon (OC) concentration in sediment simulation tests is typically high and the formation of non-extractable residues (NERs) may be significant.

- You must explain and scientifically justify the extraction procedure and solvent used obtaining a quantitative measure of NERs.
- The total amount of NER must be quantified, to demonstrate that all transformation and/or degradation products which have formed have been extracted and can be quantified. By default, total NER is regarded as non-degraded parent. 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 R.11.4.1.1.3.).
- You have the option to further characterise the types of NER to refine the P assessment. The Background note on 'Options to address NER in regulatory P assessment', published on the ECHA website provides some suggestions on the further refinement (https://echa.europa.eu/documents/10162/13632/bg_note_addressing_non-extractable_residues.pdf/e88d4fc6-a125-efb4-8278-d58b31a5d342).

e) Sterile controls

Sterile water-sediment controls must be included in the test to determine to what extent the test substance decrease is due to biotransformation or to potential abiotic losses (e.g. volatilization, formation of NERs).

ECHA notes that it is important to ensure that test conditions in the sterile controls and the active test bottles are as identical as possible. A precondition for conclusion on degradation is that other removal processes are not assessed as degradation. With this aim it is necessary to compare processes observed in sterile controls with those observed in the active test bottles under comparable test conditions.

Therefore, other test specifications of the sterile control bottles, such as the headspace volume, sampling times, analytical measurements as well as any potential causes of disturbance (such as aeration events) which may affect the distribution of the test substance or that could cause leakage, must be the same as in the active water-sediment test bottles, to ensure comparability.

OECD TG 308 does not include instructions for a sterile control. However, OECD TG 309 gives guidance on the preparation of sterile water controls as well as sterile controls containing water with sediment added in large amounts. Furthermore, ECHA notes that the OECD TG 308 test (Unnamed, 2010; ECHA, 2018) for decamethylcyclopentasiloxane (EC 208-764-9), as well as other published water-sediment degradation simulation studies (e.g. Liu et al, 2013; Shrestha et al 2016, 2020) included sterile controls and can provide guidance on the preparation of sterile controls. In these studies the sterilisation was done either by the addition of sodium azide, autoclaving or both. In addition, in another publication (Otte et al, 2018) different methods for sterilisation of marine sediment were compared.

The selection of the sterilisation method and time to perform the sterilisation in the sterile water-sediment controls, e.g. before or after the acclimation period specified in the paragraph 31 of OECD TG 308, may have an effect on the sediment properties. Based on Otte et al. (2018), thermal sterilization, gamma radiation and chemical sterilisation have all advantages and disadvantages. Considering the importance of the integrity of the sediment phase to produce meaningful results for comparison to unsterilised conditions, ECHA recommends to use methods that have the least impact on the mineral phases and the geochemistry of the sediment.

OECD TG 309 indicates that the sorption characteristics of the sediment may be altered by autoclaving. According to Otte et al (2018) autoclaving and gamma radiation lead to a large increase in dissolved organic carbon and have impacts on the mineral phase, while chemical sterilisation seems to be the method that would likely have the least impact on

the geochemistry of the sediment phase. However, it should be noted that chemical sterilisation may also affect some sediment properties, e.g. triggering changes in pH.

In conclusion, you must explain and justify the methods and procedure used for establishing the sterile controls in the study report and determine the efficiency of the sterilisation by measurements of microbial biomass. OECD TG 308 indicates that the microbial biomass of both water and sediment must be measured at post-handling, test start and test end, and mentions methods for that.

f) Full study report

You must submit the full study report, including details on the implemented method, the raw data collected, your interpretations and calculations, the consideration of uncertainties, the argumentation, your chromatograms etc. This will allow the evaluating MSCA to fully assess all the provided information, including the statistical analysis, and to clarify the concern for persistency.

A.6 Alternative approaches and proportionality of the request

Simulation studies using water, soil or sediment are able to generate data that may be suitable and necessary to obtain information that will allow to clarify whether there is a potential risk that the C16 fraction of the registered substance may contain isomers with PBT/vPvB properties. Data from these simulation studies allow to compare directly with the criteria for persistency in the REACH Annex XIII.

The request is:

- appropriate, because the test is suitable and necessary to obtain information which will allow to clarify whether the C16 fraction of the Substance contains isomers that have a half-life in water which fulfils the P or vP criteria;
- the least onerous measure, because there is no equally suitable alternative methodology available to obtain the information that would clarify the potential hazard.

The surface water compartment is considered the most relevant based on distribution modelling. According to Mackay level III model, assuming all emissions are only to water: 69–90% of C16 isomers in the Substance will distribute to the water compartment, <0.002% to soil, 9.3–30.8% to sediment and 0.44–0.82% to air.[6]

A.7 Consideration of your comments on the draft decision

You had several comments to the draft decision:

1. Concerning test strategy and new information on environmental fate and bioaccumulation of the Substance.

   You had included new information on environmental fate and bioaccumulation. You had performed modelling that indicated that the Substance would partition mainly to air where it would degrade rapidly. Hence you considered that the requested study was not necessary since it measures degradation in water. The eMSCA however has estimated using Mackay level III model in EPIsuite that the Substance partitions enough to water to warrant an OECD TG 309 study (see section A.6).

[6] Estimated using Mackay level III model in EPIsuite.

In addition you argued that the Substance was probably not B, based on a read-across from a study (Camenzuli et al, 2019) with similar alkanes, notably heptamethylnonane. Therefore, you proposed that it was not necessary to perform any additional study if the Substance does not have B-properties.

The eMSCA considered that although heptamethylnonane, based on structural similarity, could be a plausible read-across source to the Substance for this purpose, the new study by Camenzuli et al. on bioaccumulation is not considered reliable for B-assessment. There are numerous deviations from the OECD TG 305: the exposure concentration is above water solubility of the tested substance solubility (around 300 ug/L), and the BCF value might have been underestimated. Also, the concentration at T0, used to derive the kinetic BCF, was already 10 times higher than the water solubility, and at the end of the uptake phase the concentration was much higher than the water solubility. It is difficult to estimate the truly dissolved concentration measured in the study, and this uncertainty has an impact on the derived BCF.
If the aqueous exposure concentration would be replaced by the water solubility value, a BCF higher than 2000 would be obtained. The study set-up also underestimates B because for one of the substances tested, fluorantine, a BCF lower than 500 is reported, while fluorantine has already been concluded to be a vB substance. The uptake was only measured on one occasion, raising uncertainty on the k1 value. In addition, heptamethylnonane was tested as a binary mixture which might also have an impact on the BCF value. Thus an alternative approach is to look at the depuration rate constant to have an indication whether the substance indeed bioaccumulates and use this in a weight of evidence approach irrespective of the BCF value.
Based on the reported depuration constant heptamethylnonane screens as B/vB, rather than not B.

2. Concerning branching degree

   You presented new information on the production process of the Substance, which in fact precludes quite a few of the isomers that the eMSCA had thought were possible. With this new information the eMSCA agrees that the branching of the Substance was overestimated in the first decision and that quarternary C16-isomers will not be found.

3. Concerning challenges in the requested test:

   You had several comments concerning technical difficulties for the testing of the C16-fraction of the UVCB Substance. These have been resolved by changing the test substance to a single representative structure (3,4,5,6,7,8-hexamethyldecane).

4. Concerning detailed modifications and communication with the eMSCA under the development of the study:

   You commented that the establishment of a suitable test design for the Substance is very complex and challenging. We agree that testing the C16 fraction is very complex. A single representative structure will instead be used for testing. Modelling shows the importance of the water compartment for the fate of the Substance, and the pelagic OECD TG 309 test is considered to be the most relevant.

   Since the test design must be adapted, you wish to perform pre-tests and you ask to not have too strict and detailed modifications in the decision, but to have a dialogue with the eMSCA. Since the test substance now has been changed to a single substance, the issues with testing have been resolved.

5. ECHA notes that communication with the eMSCA is possible after the final decision has been issued if you wish to have a mutual discussion to clarify any additional uncertainties regarding performing of the test.

B.1 Consideration of the time needed to perform the requested studies

The deadline to provide the requested data includes the time required for developing an analytical method, conducting of the study according to the test guideline, preparation of the study report and reporting in IUCLID.

The eMSCA agrees that testing of the degradation of a UVCB substance is challenging, and a single representative structure (3,4,5,6,7,8-hexamethyldecane) is now requested.

For a simulation testing on ultimate degradation of a single representative structure (3,4,5,6,7,8-hexamethyldecane) in surface water, ECHA considers that 24 months is a sufficient time for conduct and reporting of the study.

Furthermore, you have not provided any documentary evidence from the testing facility to support your claim that an extension to 36 months would be needed.

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Appendix 2: Procedural history

On the basis of an opinion of the ECHA Member State Committee and due to initial grounds for concern relating to PBT/vPvB properties, Alkanes, C16–(branched), C20-(branched) and C24-(branched) (List number 700-992-1) (previously registered as Alkanes, C16-20-iso, EC No 292-461-1, CAS RN 90622-59-6) was included in the Community rolling action plan (CoRAP) for substance evaluation to be evaluated in 2014. The updated CoRAP was published on the ECHA website on 26 March 2014. The competent authority of Norway was appointed to carry out the evaluation.

In accordance with Article 46(1) of REACH, a substance evaluation decision was issued on 26 July 2016 requesting further information. You submitted all the requested information on 9 November 2018. The evaluating MSCA carried out the evaluation of the information in your updated registration(s) and other relevant and available information.

The evaluating MSCA considered that further information was required to clarify the PBT/vPvB properties. Therefore, it prepared a draft decision under Article 46(3) of REACH to request further information. It subsequently submitted the draft decision to ECHA on 6 November 2019.

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

Registrant(s)' commenting phase

ECHA received your comments and forwarded them to the evaluating MSCA without delay.

The evaluating MSCA took your comments, which were sent within the commenting period, into account and they are reflected in Appendix 1. The requests and the deadline were amended.

ECHA notified you of the draft decision a second time and invited you to provide comments on sections changed since your previous comments. The evaluating MSCA considered your further comments from the second consultation, and amended the deadline.

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. Subsequently, the evaluating MSCA received proposal(s) for amendment to the draft decision and modified the draft decision (see appendix 1).

ECHA referred the draft decision, together with your comments, to the Member State Committee.

ECHA invited you to comment on the proposed amendment(s). Your comments on the proposed amendment(s) were taken into account by the Member State Committee.

(i) MSC agreement seeking stage

The Member State Committee reached a unanimous agreement in its MSC-75 written procedure and ECHA took the decision according to Article 52(2) and Article 51(6) 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 3: Further information, observations and technical guidance

1. This decision does not imply that the information provided by you in the registration(s) is in compliance with the REACH requirements. The decision neither prevents ECHA from initiating compliance checks on your dossier(s) at a later stage, nor does it prevent a subsequent decision under the current substance evaluation or a new substance evaluation process once the present substance evaluation has been completed.

2. Failure to comply with the request(s) in this decision, or to otherwise fulfil the information request(s) with a valid and documented adaptation, will result in a notification to the enforcement authorities of your Member State.

3. It is the responsibility of the registrant(s) to document the necessary information on the composition of the test material. The substance identity information of the Substance and of the sample tested must enable the evaluating MSCA and ECHA to confirm the relevance of the testing for the Substance subject to substance evaluation. The isomer 3,4,5,6,7,8-hexamethyl, which has been determined to be present in the registered UVCB substance, is considered as a reasonable worst case structure, as described in more detail in Appendix I.

Appendix 4: Additional information on modelling and comparable substances

A. Modelling of P and B properties by the eMSCA

When persistency and bioaccumulation are considered together, it appears that C16 isomers with 4 branches or more may constitute a P/vP and B/vB concern as they are potentially persistent and bioaccumulative based on modelling. The results must however be treated with caution. Biodegradation of the constituents of tetrabutane has been predicted using the BIOWIN and BioHCWin programs as incorporated in the OECD toolbox version 3.3.2. Half-lives for branched petroleum compounds are, according to Rorije et al. (2012), often under-predicted in the BioHCwin model. The models contain alkanes with carbon number up to 16, and may be considered relevant for predictions for the C16 fraction of the Substance, but these are either linear or contain terminal branching. For bioaccumulation, this is also the case. The linear C16 molcule is expected to be readily metabolized in fish[7] and therefore not likely to bioaccumulate, while the highly branched isoalkane 2,2,4,4,6,8,8-heptamethylnonane has an experimental BCF of 6600. These two alkanes represent extremes in degree of branching and demonstrate that branched alkanes may be very bioaccumulative or easily metabolized, depending on branching. A combination of Biowin 2 + 3 or Biowin 3 + 6 are used to screen the persistency of chemicals for the PBT assessment.
Criteria for P are Biowin 3 < 2,2 and Biowin 2 and 6 < 0,5. No corrections were made in the BioHCWin or BIOWIN models to predict the degradability of branched compounds. However, none of the structures modelled fulfil the screening criteria for P with BioWin 3. The modelling presented here should be considered inconclusive, and further evidence is needed.

For clarity, the tentative P and B designations of the possible isomers in tetrabutane are indicated in Table 1, and for the single representative structure (3,4,5,6,7,8-hexamethyldecane) in Table 2. Both followed the PBT criteria, where P is compared to freshwater criteria (freshwater half-life 40 d), vP (freshwater half-life 60 d), B is set to BCF/BAF=2000 and vB set to BCF/BAF=5000.

Table 1 Tabular presentation of estimated P and B properties

Carbon no	Branch	Half-life in surface water (BioHCwin)	BioWin 3	BioWin 2	BioWin 6	BCF regression based	BCF Lower trophic	BCF Upper trophic	BAF Upper trophic[8]
C16	1	Not P	Not P	Not P	Not P	Not B	Not B	Not B	**Pot[9] vB**
C16	2	Not P	Not P	Not P	Not P	Not B	Not B	Not B	**Pot vB**
C16	3	Not P	Not P	Not P	Pot P	Not B	Not B	Not B	**Pot vB**
C16	4	**Borderline P (30 days)**	Not P	Pot P - Not P	Pot P	**Pot B**	Not B	Not B	**Pot vB**

[7] The experimental BCF=5011 for this substance can not be considered a reliable value, because it was determined at concentrations far above the water solubility, and was subsequently recalculated with the water solubility as exposure concentration. It should be noted that reliable BCF estimates for linear alkanes generally result in low BCF values, possibly as a consequence of extensive metabolism [e.g. Tolls & van Dijk, 2002].
[8] BAF is not part of the formal PBT criteria listed in REACH annex XIII
[9] Pot = Potential

C16	5	**Borderline P (34 days)**	Not P	Pot P - Not P	Pot P	**Pot vB**	Not B	Not B	**Pot vB**
C16	6	**Borderline P (39 days)**	Not P	Pot P	Pot P	**Pot vB**	Not B	Not B	**Pot vB**
C20	3	**Potential P**	Not P	Not P	Pot P	Not B	Not B	Not B	**Pot vB**
C20	4	**Potential P**	Not P	Not P	Pot P	Not B	Not B	Not B	**Pot vB**
C20	5	**Potential vP**	Not P	Pot P - Not P	Pot P	Not B	Not B	Not B	**Pot vB**
C20	6	**Potential vP**	Not P	Pot P - Not P	Pot P	Not B	Not B	Not B	**Pot vB**
C20	7	**Potential vP**	Not P	Pot P - Not P	Pot P	Not B	Not B	Not B	**Pot vB**
C20	8	**Potential vP**	Not P	Pot P	Pot P	Not B	Not B	Not B	**Pot vB**
C24	4	**Potential vP**	Not P	Not P	Pot P	Not B	Not B	Not B	Not B
C24	5	**Potential vP**	Not P	Not P	Pot P	Not B	Not B	Not B	Not B
C24	6	**Potential vP**	Not P	Pot P - Not P	Pot P	Not B	Not B	Not B	Not B
C24	7	**Potential vP**	Not P	Pot P - Not P	Pot P	Not B	Not B	Not B	Not B
C24	8	**Potential vP**	Not P	Pot P - Not P	Pot P	Not B	Not B	Not B	**Pot B**
C24	9	**Potential vP**	Not P	Pot P - Not P	Pot P	Not B	Not B	Not B	**Pot B**
C24	10	**Potential vP**	Not P	Pot P	Pot P	Not B	Not B	Not B	**Pot B**

Table 2: 3,4,5,6,7,8-hexamethyldecane - Tabular presentation of estimated P and B properties

Carbon no	Branch	Half-life in surface water (BioHCwin)	BioWin 2	BioWin 3	BioWin 6	BCF regression based	BCF Lower trophic	BCF Upper trophic	BAF Upper trophic[10]
C16	6	**Borderline P** (39 days)	Not P	Pot P	Pot P	**Pot vB**	Not B	Not B	**Pot vB**

Bioaccumulation

The available estimated bioaccumulation data in the registration is based on a C18 structure and as such is not reliable since C18 does not exist in the registered substance. Estimations by the eMSCA using regression based BCFBAF v3.01 suggests that fish bioconcentration factors (BCFs) may exceed 2,000 L/kg for C16 isomers with 4 branches and 5,000 L/kg for C16 isomers with 5 and 6 branches, but not for C20 and C24. However, this estimation model does not attempt to correct for metabolism. The Arnot-Gobas model for BCF (in BCFBAF v3.01), which integrates calculated whole body metabolism, shows a maximum BCF of 730 for lower trophic level for C16 isomers with 6 branches. Both models have merit, and one does not necessarily overrule the other. These models indicate that bioaccumulation may occur for some isomers, although metabolism could lead to reduced accumulation. Due to the lipophilic nature of the Substance, uptake via diet may exceed uptake via the gills. BAF values estimated by the eMSCA for upper trophic level (BCFBAF v3.01) indicate that this may be the case, with bioaccumulation factor (BAF) values above 100.000 for C16 structures, 20.000-25.000 for C20 and 1400 – 2600 for C24. Note that BAF values are not part of the formal PBT criteria listed in REACH annex XIII. However as noted in ECHA guidance for the PBT assessment, chapter R.11, page 50, the use of BAF is not excluded: "a case by case assessment based on expert judgement...is required....".

[10] BAF is not part of the formal PBT criteria listed in REACH annex XIII

Thus, the presence of isomers in the Substance that may fulfil bioaccumulation criteria in addition to potentially fulfilling persistence criteria cannot be ruled out. Dietary exposure is most likely to lead to bioaccumulation, as long as the substance is not extensively metabolized.

B. Comparable substances and substance category

Since only limited experimental data are available on the Substance itself, comparison to screening tests on other alkanes with comparable carbon numbers may be informative.

Comparison to screening tests from other hydrocarbons with comparable carbon number and registrant-performed read-across[11] show that the criterion for ready biodegradation (> 60 %) was achieved in some cases, while in other the substances were considered not readily biodegradable. The substances are all saturated hydrocarbon UVCBs and have considerable overlap with the Substance in carbon number, boiling point and partitioning coefficient.

The results from the biodegradation tests for each UVCB characterizes the biodegradability of that substance as a whole, but they do not suggest that each isomer of the UVCB is equally biodegradable. Determining the biodegradation potential of UVCBs can be challenging, as ready biodegradation test systems and study designs are not capable of distinguishing the relative contribution of the substances' isomers to the total biodegradation measured. Isomers with more branching or cyclic substructures may degrade to a lesser extent than linear and less branched isomers and the UVCB itself may still contain a certain amount of persistent isomers. Since the exact composition of these chemicals is not known, it is difficult to assess how these data can be used to support the assessment of the Substance.

OECD Category C14-C20 Aliphatic [≤2 % aromatic] Hydrocarbon Solvents

This category comprises multi-constituent aliphatic hydrocarbons with predominantly carbon number C14 to C20. Constituents in this category are hydrocarbon solvents containing straight chain (n), branched (iso) and cyclic aliphatic hydrocarbons with aromatic content of ≤ 2 %. Benzene is intentionally removed to levels less than 0.01 % and sulphur and nitrogen compounds are removed by the refining process.

A SIDS (Screening Information Dataset) Initial Assessment Profile (SIAP) has been developed for C14-C20 Aliphatic Hydrocarbon Solvents with less than 2% aromatics. Members in this Category are fully saturated hydrocarbons and have or are expected to have similar toxicokinetics, mammalian and ecological toxicological properties according to CoCAM 2011. The group is divided into three subcategories, iso-paraffins, n-paraffins and a multi-constituent subcategory. Members of the iso-paraffins subcategory are expected to demonstrate a slower rate of biodegradation than n-paraffins based on results for one of the multi-constituent isoparaffinic substances, showing a moderate extent of biodegradation (25 %) over an extended period of time of 37 days. Multi-constituent subcategory members containing aliphatic linear, branched, and/or cyclic paraffins molecules of carbon and hydrogen, predominantly in the C14 to C20 range are not

[11] Alkanes, C12-26-branched and linear, EC number 292-454-3
Hydrocarbons, C14-C20 n-alkanes <2 % aromatics, EC number 923-583-1
Hydrocarbons, C16-C20 n-alkanes, isoalkanes, cyclics, <2 % aromatics, EC number 919-029-3
C8-C26 branched and linear hydrocarbons – Distillates, EC number 481-740-5
Distillates (Fischer-Tropsch), heavy, C18-50 - branched, cyclic and linear, EC number 482-220-0

expected to be readily biodegradable.

Fate: In the SIDS of the C14-C20 aliphatic category the following is concluded for persistency: The n-paraffins sub-category members have the potential to biodegrade rapidly based on results that support their characterization as readily biodegradable. Tetrabutane can be compared to the members of the iso-paraffins subcategory, which are expected to demonstrate a slower rate of biodegradation than n-paraffins. This is based on results for one of the multi-constituent iso-paraffinic substances, which was shown not to be readily biodegradable, but did demonstrate a moderate extent of biodegradation (25%) over an extended period of time (37 days). Multi-constituent subcategory members are not expected to be readily biodegradable.

Of the 118 representative C16 structures that were initially drawn up by the eMSCA, 85 are identified by the OECD QSAR toolbox v3.3 as part of the OECD HPV category C14+ Aliphatic Hydrocarbon Solvents (≤2 % aromatics). This is based on an equation (C{H3}"*E3;C{H}{sp3}{>=11}") stating that to be identified as part of the category, the molecules must be saturated, contain at least 11 carbons, and may not contain quaternary carbons. The 33 C16 structures not identified as part of the C14+ category all contain a quaternary carbon. With the improved insight that formation of quaternary carbon is not possible with the current production process, all C16 isomers in the Substance fall within the category.
A similar comparison for C20 and C24 was not performed, as the full range of possible structures was not drawn up, but all of the suggested structures were identified as category members.