MINISTERIO
PARA LA TRANSICIÓN ECOLÓGICA
Y EL RETO DEMOGRÁFICO

HAZARD ASSESSMENT

OUTCOME DOCUMENT

for

Alkane 6

EC No 438-390-3

CAS No 151006-63-2

Member State(s): Spain

Dated: 23 January 2023

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1. HAZARD SUBJECT TO ASSESSMENT

Alkane 6 was originally selected for hazard assessment in order to clarify suspected hazard properties:

PBT/vPvB

2. OUTCOME OF HAZARD ASSESSMENT

The available information on the substance and the hazard assessment conducted has led the assessing Authority to the following considerations, as summarised in the table below.

Hazard Assessment Outcome	**Tick box**
According to the authority's assessment the substance does not have PBT/vPvB properties based on the currently available information.	X
According to the authority's assessment the substance has PBT/vPvB properties.	
According to the authority's assessment further information would be needed to confirm the PBT/vPvB properties but follow-up work is not relevant or carried out at present.	

This outcome is based on the REACH and CLP data as well as other available relevant information.

3. BASIS FOR REASONING[1]

The substance belongs to a group of substances called polyalpha olefins (PAO) which are branched, acyclic synthetic alkanes with defined molecular weights. No information on the constituents of this UVCB substance is available. Therefore, the PBT assessment has been carried out based on:

- the screening of predicted possible structures of the constituents of Alkane 6, i.e., dimers, trimers and tetramers and,
- available information on structurally related substances

Persistency

No screening tests are available for Alkane 6. Ready biodegradation tests are available for Alkane 4 and other similar substances belonging to the PAO category. There was high variation in the degradation percentage, from 0 to over 60% after 28 days, even in tests performed with the same substances. In some of the tests low bioavailability caused by the poor solubility of the substances may have caused lack of degradation, and in the OECD TG 301B tests possible volatilisation of some of the constituents cannot be excluded. The reliability of the tests cannot be evaluated due to limited information.

All test substances were UVCBs consisting of hydrogenated dimers and other oligomers of C10-C16 alpha olefins. It is difficult to draw conclusions on the degradation of individual constituents on the basis of the available ready biodegradation studies conducted on UVCB substances. In these tests, the primary degradation of the individual constituents was not

[1] Assessments of PBT properties are based on Annex XIII to the REACH Regulation.

determined. However, the relatively high degradation observed in some of the tests, even reaching pass level, suggests that at least most of the constituents of the structural similar substance Alkane 4, seem to be rapidly degradable and are not likely to be P.

Based on BIOWIN QSAR models none of the example dimer, trimer and tetramer constituents fulfils the screening criteria for P/vP according to ECHA Guidance on IR&CSA Chapter R.11. Some of the trimers and tetramers with quaternary carbons as well as dimers with branching at or close to terminal position are or are close to being considered borderline cases for screening P according to ECHA Guidance R.11.

However, based on the available information on the structures of constituents of poly alpha olefins, all constituents of Alkane 6 have at least one and most of them two or more long linear alkyl chains. These are likely to be susceptible to primary degradation through terminal or subterminal oxidation and subsequent β-oxidation.

The degradation of the side chains leads to formation of branched carboxylic acids. After the primary degradation of the side chains, most of the transformation products are of low or medium molecular weight. Therefore, they are not expected to be persistent based on BIOWIN QSARs estimations performed on hypothetical constituents and experimental data from similar structural substances.

The substance contains also low concentrations of hydrogenated monomers of linear decane (C10) and dodecane (C12) . There is no data available on ready biodegradation for these substances. Based on the available supporting experimental information on ready biodegradation on structural analogues decane (EC 204-686-4) and dodecane (EC 203-967-9), found in the ECHA dissemination site and considering the scientific articles on linear alkane degradation mentioned above in this document, these linear alkane constituents are not persistent.

Even if the route of degradation may be quite predictable, the lack of experimental data on the rate of primary degradation could result in some uncertainties, due to different stearic properties (i.e. molecular size and shape) of the constituents.

Considering all the available information in a weight of evidence assessment, it is concluded that the constituents of Alkane 6 are likely to be not persistent.

Bioaccumulation

Based on the predicted log Kow values above 4.5 and log Koa values above 5, all constituents of Alkane 6 screen potentially B/vB in aquatic and air-breathing organisms.

However, the predicted log Kow values are all above 10, which may indicate limited uptake. Also the predicted molecular diameter is high for most of the dimers and all oligomers from trimers onwards. It is noted that folding of the long linear alkyl chains could make some of the constituents more easily transferable across cell membranes. This could occur for some of the dimers and possibly for trimers, but tetramers are expected to be so big and bulky molecules that their uptake is expected to be very limited.

All BCF values predicted using the BCFBAF (v3.01) QSAR models are low, but the models have high uncertainty for substances with such a high log Kow values.

Based on the available toxicokinetic information, uptake and possible accumulation of some of the dimers or trimers of Alkane 6 in mammals cannot be fully excluded.

Alkane 6 has a very high number of different constituents. The bioaccumulation potential of the constituents may differ depending on their branching and length of the alkyl chains. Based on the high log Kow and high molecular size, the constituents are likely to have limited uptake, leading to low bioaccumulation potential. However, based on the available toxicokinetic information on rats, it seems difficult to completely remove the concern on potential B

properties of all possible dimers and trimers. Nevertheless, as the constituents are concluded to be not persistent, no further assessment on bioaccumulation potential is needed.

Toxicity

No aquatic toxicity tests are available for Alkane 6. The tests included in the dossier are performed with Alkane 4 and other members of the PAO category. These include acute tests for the three trophic levels and chronic tests for daphnia and algae.

All tests used WAFs and results are based on nominal loading rates well above the water solubility of the test substances. No effects were observed in the tests.

RAC concluded in 2018 that the similar substance Alkane 4 (mainly consisting of trimers of C12) is not expected to have chronic toxicity in aquatic organisms based on data on the category members and QSAR predictions (ECHA 2018). Consequently, the previous harmonised classification as Aq. Chronic 4 ("safety net" classification) was removed. Therefore, it seems likely that the trimers of Alkane 6 do not show aquatic chronic toxicity below the T criterion. However, it is noted that RAC did not evaluate possible differences in the toxicity of constituents or of minor constituents (e.g. dimers).

Based on the available information it is not possible to firmly conclude on T of all individual constituents

Overall conclusion:

Considering all available information in a weight of evidence assessment, it is concluded that the constituents of Alkane 6 are likely to be not persistent, the substance is considered not to fulfil the PBT/vPvB criteria of REACH annex XIII.