MINISTERIO
PARA LA TRANSICIÓN ECOLÓGICA
Y EL RETO DEMOGRÁFICO

HAZARD ASSESSMENT

OUTCOME DOCUMENT

for

EC/List number	CAS number	Substance name
418-550-9	168689-49-4	Hexadecyl 4-chloro-3-[2-(5,5-dimethyl-2,4-dioxo-1,3-oxazolidin-3-yl)-4,4-dimethyl-3-oxopentamido]benzoate

Member State(s): Spain

Dated: 23 January 2023

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initiate at a later stage. Hazard assessments and their outcomes are compiled on the basis of information available by the date of the publication of the document.

1. HAZARD SUBJECT TO ASSESSMENT

The substance covered in this document (EC 418-550-9) was 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]

Following assessment has been carried out for the Substance EC 418-550-9.

Persistence

Parent substance:

Due to the low water solubility, hydrolysis half-lives could not be determined for the Substance in an OECD 111 study. Based on HYDROWIN QSAR model predictions, the amide and ester groups of the substance are not rapidly hydrolysed, whereas the carbamate group could potentially undergo rapid hydrolysis at neutral and alkaline conditions.

AOPWIN QSAR model predicts indirect photodegradation half-life of 0.33 days for reaction with OH-radicals. However, based on the low predicted Henry's Law Constant, photodegradation in air is not considered a significant degradation route for the Substance.

In the available OECD 301B study no degradation of the Substance was observed. Therefore, the Substance screens potentially P/vP. The results of the BIOWIN QSAR models support this conclusion.

No simulation studies are available, and hence, no definitive conclusion on persistence can be drawn.

Transformation/degradation products

It is noted that the Substance is poorly soluble and the initial concentration used in the OECD 301B test was several orders of magnitude higher than the water solubility of the Substance. Therefore, it cannot be excluded that under environmental conditions some (primary)

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

degradation could occur. Based on EAWAG biodegradation pathway prediction model, the cleavage of the ester bond is a likely transformation step leading to formation of the corresponding acid and alcohol components.

Some of the potential transformation products predicted by EAWAG PPS model (with likelihood of the first transformation steps neutral) either fulfil or are borderline cases for meeting the screening criteria for potential P/vP based on BIOWIN models. Therefore, B assessment is also considered for these transformation products.

Bioaccumulation

The Substance has a high predicted log Kow (10.49). This could suggest limited bioaccumulation potential due to hindered uptake.

In the available dietary bioaccumulation study in fish, which is considered reliable with restriction by the eMSCA, the Substance was quickly depurated and low BMF values were obtained.

Therefore, it is concluded that based on the available information, the Substance is not B/vB in aquatic organisms.

Based on the predicted log Kow and log Koa values, the Substance fulfils the screening criteria for bioaccumulation potential in air-breathing animals. However, in the available OECD TG 417 toxicokinetic study, low absorption and rapid excretion of the Substance and its de-esterified metabolite were observed.

Therefore, it is concluded that the Substance is not likely to bioaccumulate in air-breathing animals, at least in mammals.

The likely degradation product, the benzoic acid formed through cleavage of the ester bond, does not screen potential B/vB based on log D value. The other potential degradation products are not likely to be B/vB either based on the predicted log Kow values and/or based on their structure.

Toxicity

Toxicity criterion was not assessed as, the Substance is not B/vB and its potential transformation/degradation products are not likely to fulfil the criteria for B/vB either.

Overall conclusion:

The Substance is potentially P/vP, but not B/vB. Some of the potential transformation/degradation products also screen potentially P/vP but none of them are likely to be B/vB, based on the available screening information.

In conclusion, the Substance is not considered to fulfil the PBT/vPvB criteria of REACH annex XIII.