



**HAZARD ASSESSMENT
OUTCOME DOCUMENT**

for

**Diphenyl(2,4,6-trimethylbenzoyl)phosphine
oxide**

EC No 278-355-8

CAS No 75980-60-8

Member State: Sweden

Dated: 8 February 2024

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1. HAZARD SUBJECT TO ASSESSMENT

Diphenyl(2,4,6-trimethylbenzoyl)phosphine oxide 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 does not have PMT/vPvM properties based on the currently available information.	
According to the authority's assessment the substance has PBT/vPvB properties.	
According to the authority's assessment the substance has PMT/vPvM 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.	
According to the authority's assessment further information would be needed to confirm the PMT/vPvM properties but follow-up work is not relevant or carried out at present.	X

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

3. BASIS FOR REASONING¹

Diphenyl(2,4,6-trimethylbenzoyl)phosphine oxide (Lucirin) is used in the following products: photo-chemicals, inks and toners, coating products, adhesives and sealants, polymers and fillers, putties, plasters, modelling clay. The substance can also be found in materials based on fabrics, textiles and apparels (e.g., clothing, mattresses, curtains, carpets, or textile toys), paper (e.g., tissues, feminine hygiene products, nappies, books, magazines, or wallpaper) and plastics (e.g., food packaging and storage, toys, or mobile phones).

Lucirin has a harmonised classification as Repr. Category 2. In September 2021, the Risk Assessment Committee (RAC) adopted its opinion on the proposal for harmonised classification and labelling (CLH) of diphenyl(2,4,6-trimethylbenzoyl)phosphine oxide as Repr. 1B by consensus². Lucirin was included in the Candidate List of substances of very high concern for Authorisation on 14 June 2023.

Persistence

Parent substance

No studies on abiotic degradation are available. HYDROWIN cannot estimate rate constants for

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

² RAC opinion, adopted 16 September 2021, CLH-O-000007023-85-01/F.

Lucirin while AOPWIN estimates a half-life of 10.7 h for phototransformation in air.

Lucirin is not ready biodegradable according to an OECD test guideline 301F test which showed 0-10% biodegradation. A biodegradation simulation test in water according to OECD test guideline 309 performed at 12°C showed that Lucirin is not persistent although very little CO₂ was formed. The half-life for primary degradation was 15-17 days and the major degradation products were according to the study report:

- Diphenylphosphinic acid (CAS No 1707-03-5)
- Diphenylphosphinous acid (CAS No 24630-80-6)
- 2,4,6-trimethylbenzoic acid (EC No 207-553-9, CAS No 480-63-7)

However, Diphenylphosphinous acid only exists in equilibrium with its tautomer Diphenyl phosphine oxide (EC No 625-671-2, CAS No 4559-70-0). The equilibrium lies far towards Diphenylphosphine oxide (see e.g. Busacca & Senanayake, 2012³). Diphenylphosphine oxide is therefore considered to be the relevant form and most likely the degradation product formed in the simulation study. Consequently, Diphenylphosphinous acid is not considered further in this assessment.

In conclusion, Lucirin does not fulfil the criteria for P/vP according to Annex XIII of Reach.

Degradation products

No experimental studies on the degradability of the three relevant degradation products are available. BIOWIN 4.11 gives the following estimates:

Substance	Biowin 2	Biowin 3	Biowin 6
Diphenylphosphinic acid	0.97	2.76	0.15
Diphenylphosphine oxide	0.98	2.80	0.18
2,4,6-trimethylbenzoic acid	0.99	2.70	0.77

It is notable that BIOWIN 2 and 6 gives very different results for both Diphenylphosphinic acid and Diphenylphosphine oxide. BIOWIN 2 indicates rapid degradation while Biowin 6 indicates slow degradation. The reason for the difference is unclear. However, both substances accumulated in the OECD 309 simulation degradation study indicating that they are poorly degradable in surface water. For 2,4,6-trimethylbenzoic acid both BIOWIN 2 and 6 indicates fast degradation. This is in contradiction with the results from the simulation study where also this degradation product accumulated indicating poor degradability. It was not possible to estimate reliable half-lives for any of the three degradation products from the simulation study data. However, persistence in the test system was indicated for all three substances and thus, all three substances screen as P/vP.

Bioaccumulation

Parent substance

The available information on bioaccumulation shows that Lucirin does not fulfil the screening criteria for B ($\log K_{OW} > 4.5$) as the available experimental $\log K_{OW}$ value is 3.1 and a QSAR value is 3.87 (KOWWIN). In addition, a fish bioaccumulation study giving a BCF of 72 further indicates that the bioconcentration factor is below the criterion for B. However, the screening criteria for terrestrial bioaccumulation ($\log K_{OW} > 2$ and $\log K_{OA} > 5$) are fulfilled as Lucirin has a predicted $\log K_{OA}$ of 12.3. Lucirin is however not persistent and may also be metabolised by

³ Busacca & Senanayake, Comprehensive Chirality, vol. 1, pp.167-216, 2012

terrestrial animals and thus is considered to have a low potential also for terrestrial bioaccumulation.

In conclusion, Lucirin does likely not meet the criteria for B/vB according to Annex XIII of REACH.

Degradation products

No experimental information is available. However, none of the three relevant degradation products screens for aquatic bioaccumulation. They all have predicted log K_{OW} -values less than the screening criterion of log K_{OW} 4.5. Furthermore, Diphenylphosphinic acid and 2,4,6-trimethylbenzoic are ionised at environmentally relevant pH (4-9) and have predicted log D at pH 7 of 0.36 and 0.31, respectively (Chemaxon log D predictor). For ionisable substances sorption to membranes or protein binding could be mechanisms for accumulation. However, none of the models included in the OECD QSAR toolbox found any alerts for protein binding for these two molecules.

Only 2,4,6-trimethylbenzoic acid screens for terrestrial bioaccumulation (predicted log K_{OW} 2.4 for the neutral molecule, predicted log K_{oa} 7.6). However, as the substance is present in its ionised form at pH 4-9 and has a predicted log D at pH7 of 0.31 it is considered to have a low potential for terrestrial bioaccumulation.

In conclusion, the degradation products do likely not meet the criteria for B/vB according to Annex XIII of REACH.

Toxicity

Parent substance

Lucirin fulfils the T criterion of Annex XIII of REACH as it has a harmonized classification for reproductive toxicity category 2 (Repro 2). Furthermore, a proposal to classify Lucirin as Repro 1B for fertility was agreed at RAC 58 (7-16 September 2021).

Whether Lucirin fulfils the T-criterion based on ecotoxicity data has not assessed.

Degradation products

No information on mammalian toxicity or ecotoxicity is available for the degradation products.

Most of the Vega and ECOSAR predictions are out of domain while the Danish models (Leadscope and SciQSAR) predicts rather low acute toxicity for all three degradation products with one exception: a 48 h EC_{50} (mg/l) for *Daphnia magna* of 0.09 mg/l.

It is therefore not possible to reliably conclude on the T-criterion for any of the degradation products.

Mobility

The CLP criteria for mobility are based on Log K_{oc} . A substance shall be considered to fulfil the mobility criterion (M) when the log K_{oc} is less than 3 and the very mobile criterion (vM) when the log K_{oc} is less than 2. For an ionisable substance, the criteria shall be considered fulfilled when the lowest log K_{oc} value for pH between 4 and 9 is less than 3 (M) or 2 (vM).

No measured log K_{oc} -values are available for Lucirin and its degradation products.

KOCWIN gives the following predictions:

Substance	Log Koc	
	MCI method	Kow method
Lucirin	2.794	2.610
Diphenylphosphinic acid	1.933	1.407
Diphenylphosphine oxide	1.759	1.434
2,4,6-trimethylbenzoic acid	1.852	1.494

Thus, Lucirin screens for M. The degradation products Diphenylphosphinic acid, Diphenylphosphine oxide and 2,4,6-trimethylbenzoic acid all screen for vM.

Overall conclusion

Parent substance

Lucirin is not persistent or bioaccumulating and thus, likely does not meet the PBT/vPvB criteria of REACH Annex XIII or the PMT/vPvM criteria of the CLP regulation.

Degradation products

P/vP: Potentially fulfilled.

B/vB: likely not fulfilled.

M/vM: screen as vM.

T: No human- or ecotoxicological data are available.

In conclusion, the degradation products do likely not meet the PBT/vPvB criteria of REACH Annex XIII. However, all three degradation products potentially fulfil the vPvM criteria of the CLP regulation.

4. TENTATIVE PLAN FOR FOLLOW-UP ACTIONS IF NECESSARY

To enable a definitive conclusion whether the degradation products of Lucirin fulfils the PMT/vPvM criteria of the CLP regulation or not, more information is necessary. To start with reliable adsorption studies according to OECD TG 106 Koc (Adsorption - Desorption Using a Batch Equilibrium Method). However, the Swedish Chemicals Agency does not wish to continue working on the substance.