



Australian Government

Department of Health and Aged Care

Australian Industrial Chemicals Introduction Scheme

2H-Pyran, 3-heptyltetrahydro-

Assessment statement (CA09812)

14 December 2023

Final



Table of contents

Contents

AICIS assessment statement (CA09812)	3
Chemical in this assessment.....	3
Reason for the assessment	3
Defined scope of assessment.....	3
Summary of assessment	3
Means for managing risk.....	6
Conclusions	6
Supporting information	7
Chemical identity	7
Relevant physical and chemical properties	7
Health hazard information.....	8
Environmental exposure	9
Environmental effects	11
Categorisation of environmental hazard.....	11
Environmental risk characterisation	12
References	13

AICIS assessment statement (CA09812)

Chemical in this assessment

Name	CAS registry number
2H-Pyran, 3-heptyltetrahydro-	854737-09-0

Reason for the assessment

An application for an assessment certificate under section 31 of the *Industrial Chemicals Act 2019* (the Act).

Certificate Application type

AICIS received the application in a Very Low to Low Risk type.

Defined scope of assessment

The chemical has been assessed:

- as a fragrance component imported into Australia at up to 1 tonne/year
- as imported in fragrance formulations at up to 1% concentration for reformulation into end use cosmetic and household products in
 - continuous action air fresheners at up to 0.3% concentration
 - fine fragrances at up to 0.1% concentration
 - instant action air fresheners at up to 0.03% concentration
 - other cosmetic and household products at up to 0.01% concentration.
- as imported in finished products for sale in:
 - continuous action air fresheners at up to 0.3% concentration
 - fine fragrances at up to 0.1% concentration
 - instant action air fresheners at up to 0.03% concentration
 - other cosmetic and household products at up to 0.01% concentration.

Summary of assessment

Summary of introduction, use and end use

The assessed chemical will not be manufactured in Australia. It will be imported either in fragrance formulations at up to 1% concentration for reformulation into finished cosmetic and household products, or in end use cosmetic and household products at up to 0.3% concentration in continuous action air freshener, at up to 0.1% concentration in fine fragrances, at up to 0.03% concentration in instant action air fresheners, at up to 0.01% concentration in other household products and leave-on and rinse-off cosmetic products.

The cosmetic and household end use products containing the chemical are proposed to be used by professional workers under industrial or non-industrial settings and by members of the general public.

Human health

Summary of health hazards

The submitted toxicological data on the assessed chemical (see **Supporting information**) indicate that the assessed chemical is:

- of low acute oral toxicity
- slightly irritating to skin and eyes
- not a skin sensitiser
- not mutagenic in a bacteria reverse mutation assay

No data on inhalation toxicity and repeated dose toxicity were submitted.

Hazard classifications relevant for worker health and safety

Based on the submitted data, the chemical does not satisfy the criteria for classification according to the *Globally Harmonized System of Classification and Labelling of Chemicals* (GHS) (UNECE 2017) for hazard classes relevant for worker health and safety as adopted for industrial chemicals in Australia.

Summary of health risk

Public

There will be widespread and repeated exposure of the public to the assessed chemical at concentrations from 0.01% to 0.3% through the use of a wide range of cosmetic and household products. The principal route of exposure will be dermal and inhalation, while incidental oral or ocular exposure is also possible. Inhalation exposure occurs particularly from the use of air care products and other products applied by spray.

The assessed chemical in neat form is slightly irritating to skin and eyes. However, these effects are not expected to occur from use of the assessed chemical at the proposed low end use concentrations in cosmetic and household products (up to 0.1%), except for continuous action air fresheners. The continuous action air fresheners are not expected to come into direct contact with skin or eyes due to designed nature of the products.

No inhalation toxicity data are provided for the assessed chemical. Due to low concentrations of the assessed chemical in the end use products, it is not expected to pose health risk through inhalation when the assessed chemical is used according to the assessed use scenarios.

No repeated dose toxicity data were provided for the assessed chemical. Considering the very low end use concentrations in cosmetics (up to 0.1%) and household products (0.3% in air fresheners), the assessed chemical is not expected to pose health risk to the public through repeated exposure from cosmetics and household products.

Overall, this assessment does not identify any risks to public health that would require specific risk management measures if the assessed chemical is introduced and used in accordance with the terms of the assessment certificate.

Workers

Reformulation workers may be incidentally exposed to the assessed chemical at up to 1% concentration during reformulation processes mainly via the dermal route, while ocular and inhalation exposures are also possible. The assessed chemical in neat form is slightly irritating to skin and eyes. However, these effects are not expected to occur during handling the assessed chemical at up to 1% concentration during the reformulation activities. To mitigate any risks to formulation workers from repeated exposure, control measures would be required (see **Means for managing risk**) to minimise the exposure. It is anticipated by the applicant that engineering controls such as enclosed and automated processes and local ventilation will be implemented where possible. Use of appropriate personal protective equipment (PPE) such as safety glasses, impervious chemical resistant gloves, protective clothing and respiratory protection will reduce worker exposure.

Professional workers in cleaning or cosmetic businesses may experience exposure via dermal, inhalation and accidental ocular exposure to the assessed chemical during the use of cleaning or cosmetic products containing the assessed chemical at up to 0.1% concentration. The professional workers may wear some PPE (including gloves, safety glasses, coveralls and face masks). If PPE is used, exposure of such workers is expected to be of a similar or lesser extent than that experienced by consumers using the same end use products containing the assessed chemical, requiring no specific risk management measures for these workers.

Environment

Summary of environmental hazard characteristics

According to domestic environmental hazard thresholds and based on the available data the assessed chemical is:

- Not Persistent (Not P)
- Bioaccumulative (B)
- Toxic (T)

Environmental hazard classification

The chemical satisfies the criteria for classification according to the GHS (UNECE, 2017) as Acute Category 1 (H400) and Chronic Category 1 (H410) based on calculated toxicity data for invertebrates and algae. Considerations were also made for the degradation of the assessed chemical.

Environmental Hazard	Hazard Category	Hazard Statement
Hazardous to the aquatic environment (acute / short-term)	Aquatic Acute 1	H400: Very toxic to aquatic life
Hazardous to the aquatic environment (long-term)	Aquatic Chronic 1	H410: Very toxic to aquatic life with long lasting effects

Summary of environmental risk

The assessed chemical will be introduced as a fragrance ingredient for use in a variety of cosmetic and household products. These uses may result in the release of the assessed chemical to sewers and to air.

The assessed chemical is readily degradable and is not persistent, has the potential for bioaccumulation and is toxic to aquatic organisms.

As the assessed chemical does not meet all three PBT criteria it is unlikely to have unpredictable long-term effects and its risk may be estimated by the risk quotient method ($RQ = PEC \div PNEC$). Based on the expected RQ values < 1 for the river and ocean compartments, it is expected that the environmental risk from the introduction of the assessed chemical can be managed.

Means for managing risk

Workers

The information in this statement should be used by a person conducting a business or undertaking at a workplace (such as an employer) to determine the appropriate controls under the relevant jurisdiction Work Health and Safety laws.

Information relating to safe introduction and use

- The following control measures should be implemented to manage the risk arising from exposure to the assessed chemical during reformulation:
 - Use of engineering controls such as
 - automated and enclosed systems where possible
 - adequate workplace ventilation to avoid accumulation of vapours, mists or aerosols
 - Use of safe work practices to
 - avoid contact with skin and eyes
 - avoid inhalation of vapours, mists or aerosols
 - Workers should wear the following personal protective equipment (PPE)
 - overalls
 - gloves
 - respiratory protection if required

Conclusions

The conclusions of this assessment are based on the information described in this statement.

Considering the means for managing risks, the Executive Director is satisfied that when the assessed chemical is introduced and used in accordance with the terms of the assessment certificate the human health and environment risks can be managed within existing risk management frameworks. This is provided that all requirements are met under environmental, workplace health and safety and poisons legislation as adopted by the relevant state or territory and the means of managing the risks identified during this assessment are implemented.

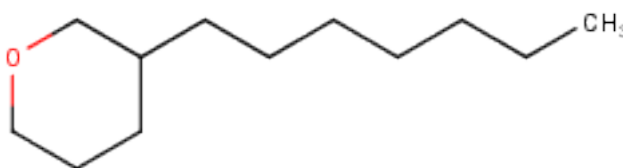
Note: Obligations to report additional information about hazards under section 100 of the *Industrial Chemicals Act 2019* apply.

Supporting information

Chemical identity

Chemical name	2 <i>H</i> -Pyran, 3-heptyltetrahydro-
CAS No.	854737-09-0
Synonyms	3-Heptyltetrahydro-2 <i>H</i> -pyran
Molecular formula	C ₁₂ H ₂₄ O
Molecular weight (g/mol)	184.32
SMILES	O1CCCC(C1)CCCCCCC
Purity	> 96 - ≤ 100%

Structural formula



Relevant physical and chemical properties

Physical form	Colourless liquid
Melting point	-38.5 °C
Boiling point	249.96 °C
Density	861 kg/m ³ at 20 °C
Vapour pressure	6.24 Pa at 25 °C (QSAR prediction [#])
Water solubility	5.02 mg/L at 25°C (QSAR prediction [*])
Ionisable in the environment?	No
log <i>K</i> _{ow}	4.7
log <i>K</i> _{oc}	3.08
Flash point	114.8 °C
Autoignition temperature	208 °C

Calculated value from iSafeRat® High Accuracy QSAR for Vapour Pressure: v1.4

*Calculated value from iSafeRat® High Accuracy QSAR for physicochemical and ecotoxicological endpoints – Version 1.9

Health hazard information

Acute toxicity

Oral

In an acute oral toxicity study (OECD TG 423), 6 female Sprague Dawley (SD) rats were administered a single dose of the assessed chemical at 2,000 mg/kg bw. No mortalities, test substance-related clinical signs or macroscopic findings were observed in any treated animals. Body weight gain appeared normal. The median lethal dose (LD50) was determined to be greater than 2,000 mg/kg bw indicating the assessed chemical is of low acute oral toxicity.

Corrosion/Irritation

Skin irritation

The assessed chemical was tested for skin irritation using 3 male albino New Zealand rabbits (OECD TG 404). A single 4-hour, semi-occluded application of the undiluted test substance to the intact skin of the rabbits produced slight to well-defined erythema (maximum score of 2) at the 1-hour observation. The mean individual erythema scores from gradings at 24, 48 and 72 hours were 2.0, 2.0, 2.0, respectively. The mean individual oedema scores from gradings at 24, 48 and 72 hours were 0.0, 0.0, 0.0, respectively. Dryness of the skin was noted in all animals from the Day 4 observation until the Day 13 observation. At the Day 14 observation, the skin of all animals appeared normal. Under the conditions of this study, the assessed chemical was slightly irritating to skin but does not meet the GHS criteria for classification.

Eye irritation

The assessed chemical was tested for eye irritation using 3 male albino New Zealand rabbits (OECD TG 405). A single application of the undiluted test substance to one eye of each rabbit produced no iridial effects. Slight to severe conjunctival irritation (maximum score of 3) was observed in the treated eye of all animals 1 hour after treatment. The mean individual conjunctival redness scores from gradings at 24, 48 and 72 hours were 2.0, 1.7, 1.3, respectively. The mean individual conjunctival oedema scores from gradings at 24, 48 and 72 hours were 1.3, 0.7, 0.7, respectively. The mean individual corneal opacity scores from gradings at 24, 48 and 72 hours were 0.0, 1.0, 0.0, respectively. All treated eyes appeared normal at the Day 7 observation. Under the conditions of this study, the assessed chemical was slightly irritating to the eyes but does not meet the GHS criteria for classification.

Sensitisation

Skin sensitisation

The skin sensitisation potential of the assessed chemical was tested using 10 guinea pigs in a guinea pig maximisation test (OECD TG 406). Following preliminary tests, an intradermal induction concentration of 25% and topical induction concentration of 100% were used, with a single topical application at 12.5% or 25% concentration used for challenge after an 18-day rest period following induction. Two animals (1 in the control group and 1 in the treated group)

were found dead on Day 10 and Day 12, respectively. Necropsy of the two animals revealed the presence of an empty stomach and an empty intestinal transit, which was considered by the study authors to be not related to the test substance application. No erythema or oedema reactions were observed after the challenge at all time points (24, 48 and 72 hours), indicating the test substance is not a skin sensitiser.

Genotoxicity

The assessed chemical was found to be non-mutagenic in a bacterial reverse mutation assay (OECD TG 471).

Environmental exposure

The assessed chemical will be imported into Australia for use as a fragrance in end use cosmetic and household products, or as a component of fragrance formulations for reformulation into end use products. Reformulation and repackaging will occur in both closed and open processes. Significant releases of the assessed chemical to the environment are not expected during reformulation, transport or storage.

The assessed chemical will be included in a wide range of products, resulting in a variety of potential exposure scenarios.

Consumer and professional end use of the assessed chemical in cosmetic and household products is expected to result in the release of the assessed chemical “down the drain” and into the sewers. Consequently, the assessed chemical will be treated at sewage treatment plants (STPs) before release to surface waters.

Use of the assessed chemical in air care products will result in direct release of the assessed chemical into the air compartment.

Environmental fate

Partitioning

The partitioning of the assessed chemical was not determined. The chemical is treated as if it is mobile in the environment as a worst-case scenario.

Degradation

Based on its measured degradation in water, the assessed chemical is categorised as not persistent.

The assessed chemical is readily biodegradable (66% degradation over 28 days in OECD TG 301D study). The 14 d window was not fulfilled, but this criterion is not applicable as the substance has multiple constituents.

Bioaccumulation

Based on its log K_{ow} value, the assessed chemical has the potential to bioaccumulate.

No bioaccumulation information was provided for the assessed chemical. The experimental partition coefficient of the assessed chemical ($\log K_{OW} = 4.7$) is above the domestic bioaccumulation threshold of $\log K_{OW} = 4.2$ (EPHC, 2009).

Predicted environmental concentration (PEC)

A predicted environmental concentration (PEC) for Australian waters was calculated assuming the maximum allowable introduction volume for environmental exposure band 2 (1,000 kg/annum) with a release reduction factor of 1 for down-the-drain style end use scenarios. Correspondingly, 100% of the introduction volume is released into sewage treatment plants (STP) over 365 days per annum. The extent to which the assessed chemical is removed from the effluent in STP processes was not calculated as a worst-case scenario.

This calculated value is conservative as not all uses of the assessed chemical are expected to result in release to STP.

The calculation of the PEC is detailed in the table below:

Total Annual Import Volume	1,000	kg/year
Proportion expected to be released to sewer	100%	
Annual quantity of chemical released to sewer	1,000	kg/year
Days per year where release occurs	365	days/year
Daily chemical release	2.74	kg/day
Water use	200	L/person/day
Population of Australia	25.423	Million
Removal within STP	0%	Mitigation
Daily effluent production	5,085	ML/day
Dilution Factor - River	1	
Dilution Factor - Ocean	10	
PEC - River	0.54	$\mu\text{g/L}$
PEC - Ocean	0.05	$\mu\text{g/L}$

Environmental effects

Effects on aquatic Life

Acute toxicity

The following calculated median effective concentration (EC50) values for the assessed chemical in model organisms across two trophic levels were provided by the applicant:

Taxon	Endpoint	Method
Invertebrate	48 h EC50 = 0.61 mg/L	<i>Daphnia magna</i> (water flea) immobilisation iSafeRat daphEC50 v1.9 Ecotox module Calculated concentration
Algae	72 h ErC50 = 1.6 mg/L	<i>Pseudokirchneriella subcapitata</i> (green algae) Growth rate iSafeRat algErC50 v1.9 Ecotox module Calculated concentration

Chronic toxicity

The following calculated no observed effect concentration (NOEC) value for the assessed chemical was provided by the applicant:

Taxon	Endpoint	Method
Algae	72 h NOErC (growth) = 0.18 mg/L	<i>Pseudokirchneriella subcapitata</i> (green algae) Growth rate iSafeRat algNOErCv1.1 Ecotox module Calculated concentration

Predicted no-effect concentration (PNEC)

The predicted no-effect concentration is expected to be greater than 0.54 µg/L.

The available standard acute ecotoxicity endpoints for this chemical are greater than 0.54 mg/L. With a conservative assessment factor of 1,000, the lowest calculable PNEC is > 0.54 µg/L.

Categorisation of environmental hazard

The categorisation of the environmental hazards of the assessed chemical according to domestic environmental hazard thresholds is presented below:

Persistence

Not Persistent (P). Based on a measured degradation study, the assessed chemical is categorised as Not Persistent.

Bioaccumulation

Bioaccumulative (B). Based on high measured log kow value, the assessed chemical is categorised as Bioaccumulative.

Toxicity

Toxic (T). Based on calculated ecotoxicity values below 1 mg/L, the assessed chemical is categorised as Toxic.

Environmental risk characterisation

Although the assessed chemical is bioaccumulative and toxic, it does not meet all three PBT criteria. It is hence unlikely to have unpredictable long-term effects (EPHC 2009). An estimate of risk may therefore be determined using the risk quotient method.

Compartment	PEC	PNEC	RQ
River	< 0.54 µg/L	> 0.54 µg/L	< 1
Ocean	< 0.05 µg/L	> 0.54 µg/L	< 0.1

The risk quotient for the aquatic compartment is expected to be less than 1. This is based on a conservative PEC, assuming 100% release of 1 tonne/annum to STPs and no removal from the aqueous stream during STP processes, and a conservative PNEC based on an assessment factor of 1,000 and acute aquatic toxicity endpoints for the chemical that each exceed 0.54 mg/L.

Therefore, based on the expected RQ < 1 the assessed chemical is not expected to pose a significant risk to the environment. As such, the environmental risks associated with the assessed chemical can be managed.

References

EPHC (2009) Environment Protection and Heritage Council, Environmental Risk Assessment Guidance Manual for industrial chemicals, Prepared by: Chris Lee-Steere Australian Environment Agency Pty Ltd, February 2009. ISBN 978-1-921173-41-7

UNECE (United Nations Economic Commission for Europe) (2017). Globally Harmonized System of Classification and Labelling of Chemicals (GHS), Seventh Revised Edition. UNECE.

