Australian Government
Department of Health
Australian Industrial Chemicals Introduction Scheme

Cashmeran (4H-inden-4-one, 1,2,3,5,6,7-hexahydro-1,1,2,3,3-pentamethyl-)

Evaluation statement

14 September 2021

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AICIS evaluation statement

Subject of the evaluation

4H-inden-4-one, 1,2,3,5,6,7-hexahydro-1,1,2,3,3-pentamethyl- (cashmeran)

Chemical in this evaluation

Name	CAS Registry Number
4H-Inden-4-one, 1,2,3,5,6,7-hexahydro-1,1,2,3,3-pentamethyl-	33704-61-9

Reason for the evaluation

The Evaluation Selection Analysis indicated a potential risk to the environment.

Parameters of evaluation

The chemical in this evaluation has been evaluated for its risks to the environment according to the following parameters:

- default domestic introduction volume of 100 tonnes
- industrial uses listed below in the 'Summary of Use' section
- expected emission into sewage treatment plants (STPs) due to consumer
- commercial use.

Summary of evaluation

Summary of introduction, use and end use

Based on international use information, the chemical in this evaluation is used as a fragrance in:

- personal care products
- air care products
- cleaning and furniture care products
- laundry and dishwashing products
- automotive care products.

There is no information available on the domestic use volume of this substance. Data from international jurisdictions indicate that it is used in the European Union (EU) at up to 100 tonnes per year, and in the USA at up to 454 tonnes (1 000 000 lb) per year.

Environment

Summary of environmental hazard characteristics

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

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

Environmental hazard classification

The chemical satisfies the criteria for classification according to the Globally Harmonized System of Classification and Labelling of Chemicals (GHS) for environmental hazards as follows. This does not consider classification of physical hazards and health hazards.

Environmental Hazard	Hazard Category	Hazard Statement
Acute Aquatic	Category 2	H401: Toxic to aquatic life
Chronic Aquatic	Category 2	H411: Toxic to aquatic life with long-lasting effects

Summary of environmental risk

Cashmeran is a fragrance chemical expected to have industrial uses in Australia. This chemical may be released to the aquatic environment in the treated effluent from sewage treatment plants as a result of its use.

Cashmeran is persistent, not bioaccumulative, and not toxic according to domestic categorisation criteria. The expected concentrations of cashmeran in domestic surface waters are below the level of concern (RQ <1). The industrial use of this chemical is; therefore, unlikely to be of high risk to the environment.

Conclusions

The conclusions of this evaluation are based on the information described in the statement. Obligations to report additional information about hazards under Section 100 of the *Industrial Chemicals Act 2019* apply.

The Executive Director is satisfied that the identified 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.

Supporting information

Rationale

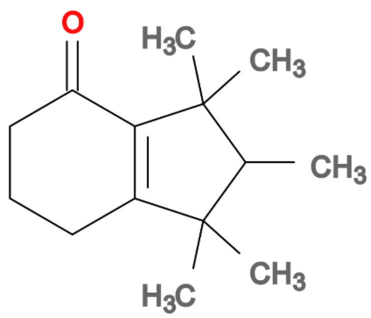
This evaluation considers the environmental risks associated with the industrial uses of cashmeran, a synthetic polycyclic musk that is used as a fragrance chemical.

Fragrance ingredients are ubiquitous components of numerous classes of formulated products including cosmetics, personal hygiene products, and various household cleaning agents. These products are released into sewers nationwide as a normal part of their use pattern. Consequently, the use of cashmeran in these products has significant potential to result in environmental exposure, through a common pathway involving release of the chemicals in the treated effluents and biosolids produced by sewage treatment plants (STPs).

The Evaluation Selection Analysis (ESA) of cashmeran highlighted potential persistence and toxicity hazard characteristics, which are of concern for the environment. This evaluation includes further refinement of the risk characterisation of cashmeran and a more in-depth assessment of the available environmental hazard and exposure information for this chemical.

Environmental risks resulting from the use of other polycyclic musks as fragrance ingredients in Australia have previously been assessed under the Inventory Multi-tiered Assessment and Prioritisation (IMAP) Framework established by the Scheme, formerly the known as the National Industrial Chemicals Notification and Assessment Scheme (NICNAS). Environment Tier II assessments are available for Tonalide and Related Polycyclic Musks (NICNAS, 2016) and Celestolide and Related Polycyclic Musks (NICNAS, 2017).

Chemical identity

Synonyms	cashmeran DPMI musk indanone indomuscone 6,7-dihydro-1,1,2,3,3-pentamethyl-4(5*H*)-indanone dihydro pentamethylindanone
Structural formula	

Molecular formula	$C_{14}H_{22}O$
Molecular weight (g/mol)	206.32
SMILES	CC1C(C2=C(C1(C)C)C(=O)CCC2)(C)C
Chemical description	N/A

Relevant physical and chemical properties

Measured and calculated physical and chemical property data for cashmeran are presented below (REACH, 2020; US EPA, 2017a):

Physical form	Solid
Melting point	27 °C (exp.)
Boiling point	220 °C (decomposition) (exp.)
Vapour pressure	1 Pa (25 °C) (exp.)
Water solubility	49.1 mg/L (20 °C) (exp.)
Henry's law constant	1.44 Pa·m^3/mol (calc.)
Ionisable in the environment?	No
pK_a	-
log K_{ow}	4.2 (20 °C) (exp.)

Introduction and use

Australia

No specific Australian use, import, or manufacturing information has been identified.

Based on information in the public domain, cashmeran is available for use in Australia as a fragrance ingredient (Australian Botanical Products, 2017).

International

Available information indicates that cashmeran is used as a fragrance ingredient in a range of consumer products worldwide.

The total registered use volume of cashmeran in the European Union (EU) is 10–100 tonnes per annum (REACH, 2020). In the Nordic countries, the average total use volume from

2014–2018 was 2.56 tonnes per annum (Nordic Council of Ministers, 2020). A maximum of 454 tonnes of cashmeran was produced annually (<1 000 000 lbs) from 2012–2015 in the United States of America (USA) (US EPA, 2016).

Cashmeran is identified as a fragrance compound on the International Fragrance Association (IFRA) Transparency List (IFRA, 2016), and on the European Commission Cosmetic Ingredient (CosIng) database (European Commission, 2020).

Cashmeran is used in washing and cleaning products, furniture care products, automotive care products, polishes and waxes, air fresheners and biocides. It is also used in cosmetics and personal care products, such as soaps, moisturiser, deodorants, and perfumes (REACH, 2020; US EPA, 2014).

In a study conducted in Portugal, cashmeran was present in 60% of the 140 personal care products sampled, with an average concentration of 125 micrograms per gram (µg/g) (Homem, et al., 2015). In Spain, cashmeran was identified in a moisturiser (17.5 µg/g), aftershave (422 µg/g), and deodorant (180 µg/g) out of the 26 personal care products sampled (Llompart, et al., 2013).

Cashmeran may only be used in limited concentrations in certain cosmetic types due to dermal sensitisation and systemic toxicity concerns (IFRA, 2019).

Existing Australian regulatory controls

Environment

The industrial use of the chemical is not subject to any specific national environmental regulations.

International regulatory status

United Nations

The chemical is not currently identified as a persistent organic pollutant (UNEP, 2001), an ozone depleting substance (UNEP, 1987), or hazardous substance for the purpose of international trade (UNEP & FAO, 1998).

Environmental exposure

Cashmeran is known to be used as a fragrance ingredient internationally in consumer products, such as cosmetics, air fresheners, personal hygiene products, and various household cleaning agents. The formulation of such products on the Australian market is assumed to not differ significantly from those international products. Therefore, cashmeran is expected to be found in a range of household and commercial products available for use in Australia.

Chemicals used in cosmetics, personal hygiene and cleaning products are typically emitted to sewers in wastewater following consumer use. Depending on degradation and partitioning processes of chemicals in sewage treatment plants (STPs), some fraction of the quantity of chemicals in waste water entering STPs can be emitted to the air compartment, to rivers or oceans in treated effluent, or to soil through application of biosolids to agricultural land

(Struijs, 1996). The emissions of cashmeran to environmental surface waters and soils are considered as part of this evaluation.

The use of cashmeran in Australia is supported by a domestic environmental monitoring study which identified the chemical in wastewater influent at a sewage treatment plant in Sydney (Wang and Khan, 2014).

Environmental fate

Partitioning

Cashmeran is expected to partition into the water compartment when released into the environment.

Cashmeran is a volatile neutral organic chemical that is moderately soluble in water. The calculated Henry's law constant for cashmeran is 1.44 $Pa \cdot m^3/mol$, indicating the chemical is moderately volatile from water and moist soil. The soil adsorption coefficient (log K_{OC} = 2.3) suggests cashmeran has medium mobility in soil (REACH, 2020).

Calculations with a standard multimedia partitioning (fugacity) model, assuming equal and continuous distributions to air, water and soil compartments (Level III output), predict that cashmeran will partition to the soil compartment (83%) and the water compartment (16%) (US EPA, 2017a). With sole release into the water compartment, the chemical will predominantly remain in the water compartment (95%).

Degradation

Cashmeran is not expected to biodegrade rapidly in the environment.

Cashmeran is not readily biodegradable based on a study conducted in accordance with the OECD Test Guideline (TG) 301C (MITI) standard test. No mineralisation of cashmeran was observed, with 0% biodegradation by biological oxygen demand (BOD) measured over 28 days. After 28 days, 99% of the test substance concentration was still present (REACH, 2020).

Cashmeran is not expected to hydrolyse in water as it lacks readily hydrolysable functional groups. Cashmeran will undergo rapid photo-oxidation by hydroxyl radicals in the atmosphere, with a calculated half-life of 1.2 hours (US EPA, 2017a).

Bioaccumulation

Cashmeran has a low potential to bioaccumulate in aquatic life.

The measured octanol-water partition coefficient of cashmeran meets the domestic categorisation threshold for bioaccumulation hazards in aquatic organisms (log K_{OW} ≥4.2), indicating potential for bioaccumulation (EPHC, 2009).

Cashmeran has a low potential to bioconcentrate in fish. A study conducted in accordance with OECD TG 305 reported a lipid-normalised bioconcentration factor (BCF) value of 157 L/kg wet weight in *Cyprinus carpio* (carp) (REACH, 2020). This value is below the domestic categorisation threshold for bioconcentration in aquatic organisms (BCF ≥2000) (EPHC, 2009).

Cashmeran has been detected in polar bear liver samples from Greenland at low concentrations (Vorkamp, et al., 2004). Of two samples, one contained cashmeran at below the limit of quantification (<5 nanograms per gram wet weight (ng/g ww)). The other sample was analysed in duplicate, finding cashmeran once at 5.5 ng/g ww and once below the limit of quantification. There are insufficient data available to determine if the detection of cashmeran in these samples is due to biomagnification, or from other more direct exposure sources.

Cashmeran has been detected in blue mussels at up to 1140 ng/g lipid weight (lw) (Mogensen, et al., 2004). These relatively high concentrations may have been due to an industrial source of musk substances near the sampling location in Sweden. Cashmeran was not detected in mussel samples from other locations in the study (18 of 20 total samples). Cashmeran has also been found in fish samples from European locations at concentrations from 6.1–9.11 ng/g dry weight (dw) (Cunha, et al., 2015).

Environmental transport

Cashmeran is not expected to undergo long range transport based on its short, calculated half-life in the atmosphere.

Predicted environmental concentration (PEC)

The concentration of cashmeran in Australian river water is estimated to be 0.033 micrograms per litre (µg/L) based on domestic monitoring data. A maximum concentration of 0.17 µg/L, based on international STP monitoring, is taken as a worst-case estimate. The concentration of cashmeran in Australian agricultural soils amended with biosolids is predicted to be 2.5 micrograms per kilogram dry weight (µg/kg dw).

A riverine concentration of 41.2 µg/L was calculated using standard exposure modelling for the release of chemicals to surface water from STPs and an assumed annual introduction volume for cashmeran of 100 tonnes (Struijs, 1996).

Domestic and international monitoring data indicate this may overestimate typical environmental concentrations. Raw wastewater obtained from a municipal sewer in Sydney returned an average cashmeran concentration of 33 nanograms per litre (ng/L) (Wang and Khan, 2014). This value is conservatively used as representative of surface water concentrations in Australia in the absence of monitoring data for cashmeran in treated effluent obtained after typical sewage treatment processes.

These domestic measured concentrations for cashmeran are consistent with concentration ranges measured in STP influent and effluent internationally. Influent concentrations in the range of 15.7–260 ng/L have been reported, with effluent concentrations in the range of 27.1–170 ng/L found after primary or secondary treatment (Clara, et al., 2011; Ramírez, et al., 2011; Smyth, et al., 2007).

Concentrations of cashmeran in biosolids in the range of 1.7–1450 µg/kg dw have been measured internationally (Clara, et al., 2011; Herren and Berset, 2000; Mogensen, et al., 2004). Mean and median concentrations of 328 and 287 µg/kg dw respectively were determined in a literature review of biosolids contaminants (Langdon, et al., 2010).

The calculated cashmeran concentration in soil amended with biosolids is 2.5 µg/kg dw based on the mean international measured biosolid concentration (328 µg/kg dw), typical biosolids application rates and a soil bulk density of 1300 kilograms per cubic metre (EPHC, 2009).

Environmental effects

Effects on aquatic Life

Acute toxicity

The following measured and calculated median lethal concentration (LC50), absolute lethal concentration (LC100), and median effective concentration (EC50) values for model organisms across three trophic levels exposed to cashmeran are presented below (REACH, 2020; US EPA, 2017b):

Taxon	Endpoint	Method
Fish	48 h LC100 ≤3 mg/L	Experimental *Oryzias latipes* (Japanese rice fish) Japanese Industrial Standard K0102-1998-71 Semi-static
	96 h LC50 = 4.4 mg/L	Calculated ECOSAR Vinyl/allyl/propargyl ketones class
Invertebrate	48 h EC50 = 1.5 mg/L	Experimental *Daphnia magna* (water flea) OECD TG 202 Immobilisation Static
Algae	96 h EC50 = 1.35 mg/L	Calculated ECOSAR Vinyl/allyl/propargyl ketones class

An acute algal ecotoxicity study conducted according to the OECD TG 201 with static renewal over 72 hours is available (REACH, 2020). Test substance concentration monitoring found large decreases (75–90% disappearance) from the nominal concentrations of the test substance over the duration of the test. Therefore, this study is not considered reliable for the purpose of this hazard assessment.

The acute fish ecotoxicity endpoint given in the table above is from a study conducted with semi-static renewal over 96 hours, though the test substance concentration was not measured (REACH, 2020). Therefore, there is potential for large decreases of the test substance concentration over the timeframe of this study as seen in the algal study above, which limits its reliability. This study found 0% mortality at all test concentrations over 96 hours up to a nominal test concentration of 1.5 mg/L. At the highest test concentration of 3 mg/L, 100% mortality was observed after only 48 hours. This study summary records a 96 h LC50 of 2.12 mg/L, which is not considered reliable due to the lack of an appropriate dose-response curve. Instead, a 48 h LC100 ≤3 mg/L is adopted. This value indicates that the calculated fish 96 h LC50 of 4.4 mg/L underestimates the acute toxicity to fish.

Effects on sediment dwelling life

Toxicity data for sediment-dwelling organisms were not identified for cashmeran.

Effects on terrestrial life

Cashmeran is not expected to cause serious harm through oral exposure. Further information on the effects of the chemical on terrestrial organisms can be found in the Human Health IMAP Tier II assessment for cashmeran (NICNAS, 2019).

Predicted no-effect concentration (PNEC)

The freshwater aquatic PNEC for cashmeran is 1.35 µg/L.

A PNEC of 1.35 µg/L was derived from the calculated algal ecotoxicity endpoint (72 h EC50 = 1.35 mg/L) using an assessment factor of 1000. This conservative assessment factor was selected as there are reliable acute ecotoxicity data available for only one trophic level, and additional ecotoxicity data for another trophic level indicating the potential for high acute toxicity to fish.

Categorisation of environmental hazard

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

Persistence

Persistent (P). Based on results from a standard biodegradability test that showed no evidence of biodegradation, cashmeran is categorised as Persistent.

Bioaccumulation

Not Bioaccumulative (Not B). Based on low measured bioconcentration factor in fish, cashmeran is categorised as Not Bioaccumulative.

Toxicity

Not Toxic (not T). Based on calculated and measured ecotoxicity values above 1 mg/L, cashmeran is categorised as not Toxic.

GHS classification of environmental hazard

Based on the available data, cashmeran is classified as Acute Aquatic Category 2 (H401) and Chronic Aquatic Category 2 (H411) under the Globally Harmonised System of Classification and Labelling of Chemicals (GHS) (UNECE, 2017).

Cashmeran is not rapidly degraded and chronic aquatic toxicity data are not available. Hence, according to the GHS guidance on classification of aquatic hazards, the long-term aquatic hazard of this chemical may be based on the acute ecotoxicity endpoints. In this case, the long-term aquatic hazard of cashmeran was classified based on the measured acute invertebrate ecotoxicity endpoint.

Environmental risk characterisation

Based on the PEC and PNEC values determined above, the following Risk Quotient (RQ = PEC ÷ PNEC) has been calculated for release into rivers:

PEC (µg/L)	PNEC (µg/L)	RQ
0.033	1.35	0.024

An RQ less than 1 indicates that cashmeran is not expected to pose an unreasonable risk to the environment based on the estimated emissions, as environmental concentrations are below the levels likely to cause harmful effects. At the worst-case environmental concentration of 0.17 µg/L, the RQ still does not exceed 1.

Insufficient data are available to characterise the risk posed by the release of this chemical to the soil compartment. However, the chemical is not expected to remain in soil based on its mobility and volatility.

Uncertainty

This evaluation was conducted based on a set of information that may be incomplete or limited in scope. Some relatively common data limitations can be addressed through use of conservative assumptions (OECD, 2019) or quantitative adjustments such as assessment factors (OECD, 1995). Others must be addressed qualitatively, or on a case-by-case basis (OECD, 2019).

The most consequential areas of uncertainty for this evaluation are:

- There are insufficient ecotoxicity data to fully characterise the acute and chronic toxicity of this chemical to aquatic, sediment or soil-dwelling organisms. Additional reliable ecotoxicity data may; therefore, change the outcome of the evaluation.
- The chemical is categorised as persistent based on the results of one ready biodegradability test, which are designed to be stringent. Additional reliable ready biodegradability or inherent biodegradability test data may; therefore, change the outcome of the evaluation.

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