Australian Government
Department of Health
Australian Industrial Chemicals Introduction Scheme

Ethanone, 1-(2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-1H-3a,7-methanoazulen-5-yl)-, [3R-(3.alpha.,3a.beta.,7.beta.,8a.alpha.)]- (acetyl cedrene)

Evaluation statement

30 May 2022

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AICIS evaluation statement

Subject of the evaluation

Ethanone, 1-(2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-1H-3a,7-methanoazulen-5-yl)-, [3R-(3.alpha.,3a.beta.,7.beta.,8a.alpha.)]- (acetyl cedrene)

Chemicals in this evaluation

Name	CAS registry number
Ethanone, 1-(2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-1H-3a,7-methanoazulen-5-yl)-, [3R-(3.alpha.,3a.beta.,7.beta.,8a.alpha.)]-	32388-55-9
Ethanone, 1-(2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-1H-3a,7-methanoazulen-5-yl)-	68039-35-0

Reason for the evaluation

Evaluation Selection Analysis indicated a potential environmental risk.

Parameters of evaluation

This evaluation considers the environmental risks associated with the industrial uses of acetyl cedrene (CAS No. 32388-55-9). Acetyl cedrene is a defined isomer of methyl cedryl ketone (CAS No. 68039-35-0) and as such this chemical has also been included in this evaluation. These chemicals have been evaluated for their risks to the environment according to the following parameters:

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

Summary of evaluation

Summary of introduction, use and end use

The chemical, acetyl cedrene, has reported industrial and professional use in Australia as a rubbing compound in marine applications. The chemical is also used as a fragrance ingredient.

Based on international use information, acetyl cedrene is used as a fragrance ingredient in the following products:

Personal care products:

- air freshener products

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

There is no information available on the domestic use volume of acetyl cedrene. Reported volumes from international jurisdictions indicate that it is used in the in the EU at up to 10 000 tonnes per year, and in the USA at up to 226.6 tonnes (500 000 lb) per year.

No current domestic or international use or introduction information was identified for methyl cedryl ketone. It does not appear to have widespread industrial use.

Environment

Summary of environmental hazard characteristics

According to domestic environmental hazard thresholds and based on the available data acetyl cedrene and methyl cedryl ketone are:

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

Environmental hazard classification

These chemicals satisfy the criteria for classification according to the Globally Harmonized System of Classification and Labelling of Chemicals (GHS) for environmental hazards (UNECE 2017). This evaluation does not consider classification of physical hazards and health hazards.

Environmental Hazard	Hazard Category	Hazard Statement
Acute Aquatic	Acute aq. – Cat. 1	H400: Very toxic to any aquatic life
Chronic Aquatic	Acute aq. – Cat. 1	H410: Very toxic to any aquatic life with long lasting effects

Summary of environmental risk

Acetyl cedrene 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 pattern.

Acetyl cedrene is persistent, not bioaccumulative, and toxic according to domestic categorisation criteria. The persistence finding is conservative, based on a lack of observed ultimate biodegradation in the water compartment. The expected concentrations of acetyl cedrene 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.

Methyl cedryl ketone is a close structural analogue of acetyl cedrene and is expected to have similar hazard characteristics. It is not expected to be present in the Australian environment at concentrations approaching the level of concern based on its apparent lack of widespread industrial use.

Conclusions

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

The Executive Director is satisfied that the identified environmental 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.

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

Supporting information

Rationale

This evaluation considers the environmental risks associated with the industrial uses of acetyl cedrene and methyl cedryl ketone, two closely related synthetic fragrances. The evaluation of these chemicals has been conducted as a group because of their structural similarity and their known or potential applications as synthetic fragrances. While common names for these chemicals appear different, the structural similarity is very close, with acetyl cedrene being a defined isomer of methyl cedryl ketone.

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 acetyl cedrene and methyl cedryl ketone 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 acetyl cedrene highlighted potential persistence, bioaccumulation and toxicity (PBT) hazard characteristics, which are of a high concern for the environment. This evaluation includes a more in depth assessment of the available environmental hazard and exposure information for both acetyl cedrene and its structural analogue, methyl cedryl ketone, in order to refine the screening risk characterisation.

Environmental risks resulting from the use of other synthetic fragrance ingredients in Australia have previously been assessed under the Inventory Multi-tiered Assessment and Prioritisation (IMAP) framework established by the former 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

The chemical represented by CAS No. 68039-35-0 is known as methyl cedryl ketone. While its structure has several chiral centres, the stereochemistry of this substance is not defined in the Australian Inventory of Industrial Chemicals (the Inventory).

The chemical represented by CAS No. 32388-55-9 will be referred to in this Evaluation as acetyl cedrene, though it is also known as methyl cedryl ketone. Acetyl cedrene is a single defined stereoisomer of methyl cedryl ketone (CAS No. 68039-35-0). Of the two chemicals, acetyl cedrene appears to be in much more widespread industrial use.

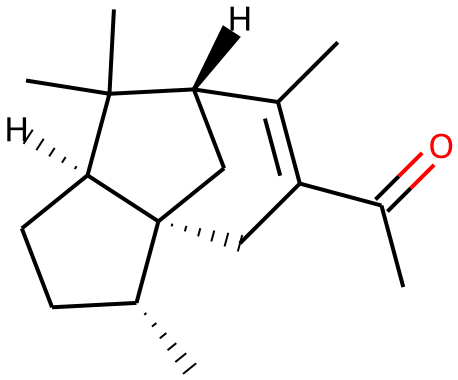
Acetyl cedrene is manufactured by the acetylation of alpha-cedrene, which is a common sesquiterpene component of cedarwood oil (CAS No. 8000-27-9). The typical manufacturing process uses cedarwood oil as the feedstock; therefore, significant impurities are created in the resulting technical mixture from the other natural components of cedarwood oil.

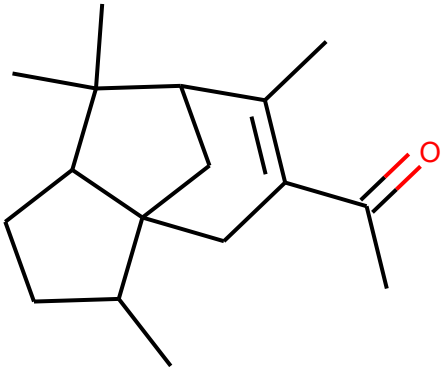
Cedarwood oil is a substance of unknown, variable composition, complex reaction products, or of biological origin (UVCB). Its composition varies depending on a number of factors, but it typically comprises primarily alpha-cedrene (2–58%), beta-cedrene (1–8%), thujopsene (5–

82%), cuparene (0.1–12.5%), cedrol (2–73%) and widdrol (0.1–17%) (CAS Nos. 469-61-4, 546-28-1, 470-40-6, 16982-00-6, 77-53-2 and 6892-80-4) (Adams 1991).

Virginia cedarwood oil (*Juniperus virginiana)* appears to be the most commonly used feedstock for the production of fragrances (NTP 2002). Available studies have identified significant quantities of alpha cedrene in Virginia cedarwood oil compared to other species (Baker et al. 2018; NTP 2002).

Purified acetyl cedrene is solid whereas the technical mixture is a liquid. The reported purity of technical mixtures of acetyl cedrene is in the range of 65–85%. The remaining 15–35% comprises acetylated isomers of cedarwood oil components and structural isomers of acetyl cedrene that are by-products of the synthetic procedure (Kamounah et al. 2011; Paknikar et al. 2017; REACH).

CAS No.	32388-55-9
Chemical name	Ethanone, 1-(2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-1H-3a,7-methanoazulen-5-yl)-, [3R-(3.alpha.,3a.beta.,7.beta.,8a.alpha.)]-
Synonyms	acetyl cedrene 9-Acetyl-8-cedrene lixetone vertofix methyl cedryl ketone
Structural formula	
Molecular formula	$C_{17}H_{26}O$
Molecular weight (g/mol)	246.4
SMILES	C[C@H]1[C@@]23[C@](C(C)(C)[C@@H](C2)C(C)=C(C(C)=O)C3)(CC1)[H]
Chemical description	-

CAS No.	68039-35-0
Chemical name	Ethanone, 1-(2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-1H-3a,7-methanoazulen-5-yl)-
Synonyms	methyl cedryl ketone lixetone vertofix couer 1H-3a,7-Methanoazulene, ethanone deriv. (ZCI) 9-Acetyl-2,6,6,8-tetramethyltricyclo[5.3.1.01,5]undec-8-ene
Structural formula	
Molecular formula	$C_{17}H_{26}O$
Molecular weight (g/mol)	246.4
SMILES	CC1CCC2C13CC(C2(C)C)C(=C(C3)C(=O)C)C
Chemical description	-

Relevant physical and chemical properties

Measured and calculated physical and chemical property data for acetyl cedrene are presented below (REACH; US EPA 2017):

Chemical	Acetyl cedrene
Physical form	Solid
Melting point	92 °C (calc.)
Boiling point	307 °C (calc.)
Vapour pressure	250 Pa at 25 °C (exp.)

Water solubility	6 mg/L at 23 °C (exp.)
Henry's law constant	14.8 Pa·m^3/mol (calc.)
Ionisable in the environment?	No
pKa	N/A
log K_{ow}	5.9 (exp.)

The measured physical and chemical property data for acetyl cedrene was for the technical mixture, containing the major component (65–85%) and impurities (15–35%). The octanol-water partition coefficients (log K_{OW} = 5.6, 5.8 and 5.9) and soil adsorption coefficients (log K_{OC} = 3.5, 4.1, 4.3, 4.4 and 5.1) measured peak values relate to the different components in the technical mixture (REACH). The measured log K_{OW} of 5.9 and log K_{OC} of 5.1 correspond to the peak value of acetyl cedrene, the major component of the technical mixture.

Detailed information is not available on the nature of the test substance used for measurements of the physical and chemical properties, and other standard tests on environmental hazard characteristics of acetyl cedrene. In some cases, how the nature of the test material has affected the outcome of the test is not known and is a source of uncertainty in this evaluation.

No data were available for methyl cedryl ketone. Since acetyl cedrene is a component of, and structurally very similar to, methyl cedryl ketone, acetyl cedrene is considered a suitable read-across analogue for determination of the physical and chemical properties and hazard characteristics of methyl cedryl ketone.

Introduction and use

Australia

Acetyl cedrene has reported industrial and professional use as a rubbing compound in marine applications.

Based on information in the public domain, acetyl cedrene is available for use in Australia as a fragrance ingredient (ABP 2017).

International

Available information indicates that acetyl cedrene is used in high volumes as a fragrance ingredient in a range of consumer products worldwide.

The total registered use volume for acetyl cedrene in the European Union (EU) is 1000–10 000 tonnes per annum (REACH). In the United States of America (USA) acetyl cedrene is listed as a high production volume chemical (US EPA 2020a), with an annual use volume of 45–226.6 tonnes (US EPA 2016). In the Nordic countries, the average annual use volume over a five year period from 2015–2019 was 7.66 tonnes per year (SPIN).

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

Acetyl cedrene is used in absorbents, air fresheners, automotive care products, washing and cleaning products, polishes and waxes and biocides. It is also used in cosmetics and personal care products, such as soaps, moisturiser, deodorants, and perfumes (REACH; US EPA 2021).

In a study conducted in the US, acetyl cedrene was identified to have concentrations of 0.02–0.8% in soap, detergent, lotion and perfume products (Food and Cosmetics Toxicology, 1975). The Consumer Product Information Database (CPID) reports concentrations of acetyl cedrene in personal care products (0.1–1.5%), washing and cleaning products (0.1–1.5%) and automotive care products (0.1–10%) (DeLima Associates).

Acetyl cedrene has a non-industrial use as an inert ingredient in pesticide products (US EPA 2021). The use of this chemical as a pesticide additive is beyond the scope of this assessment.

No specific international use, import or manufacturing information has been identified for methyl cedryl ketone. It is listed as a perfuming agent on the European Commission's CosIng database (EC), and on the IFRA Transparency List (IFRA). However, it is not registered under the EU REACH legislation and is 'inactive' on the US Environmental Protection Agency (US EPA) chemical substance inventory (ECHA 2020b; US EPA 2020b). Methyl cedryl ketone does not appear to have widespread industrial use internationally.

Existing Australian regulatory controls

Environment

The industrial use of acetyl cedrene and methyl cedryl ketone is not subject to any specific national environmental regulations.

International regulatory status

United Nations

Acetyl cedrene and methyl cedryl ketone are not currently identified as persistent organic pollutants (UNEP 2001), ozone depleting substances (UNEP 1987), or hazardous substances for the purpose of international trade (UNEP & FAO 1998).

European Union

Acetyl cedrene is present on the Community Rolling Action Plan (CoRAP) list for an eventual evaluation to be conducted by a member state of the EU (ECHA 2020a). It was listed on the CoRAP after fulfilling the potential endocrine disruption, suspected PBT/vPvB and exposure criteria.

Environmental exposure

Acetyl cedrene is known to be used as a fragrance ingredient internationally in consumer products, such as cosmetics, air fresheners, personal care 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, acetyl cedrene is expected to be found in a range of household and commercial products available for use in Australia.

Chemicals used in personal care and household cleaning products are typically emitted to wastewater following consumer uses. Depending on degradation and partitioning processes of chemicals in sewage treatment plants (STPs), some fraction of the quantity of chemicals in wastewater entering STPs can be emitted to the air compartment, to rivers or oceans from treated effluent, or to soil through application of biosolids to agricultural land (Struijs, 1996). The emissions of acetyl cedrene and methyl cedryl ketone to environmental surface waters, sediment, and soils are considered as part of this evaluation.

Environmental fate

Partitioning

Acetyl cedrene partitions to air, water, and soil when released into the environment.

Acetyl cedrene is a highly volatile neutral organic chemical that is slightly soluble in water. The calculated Henry's law constant for acetyl cedrene is 14.8 Pa·m^3/mol, indicating the chemical is moderately volatile from water and moist soil. Acetyl cedrene is a lipophilic chemical with a measured log K_{OW} of 5.9 and a soil adsorption coefficient of log K_{OC} = 5.1, that indicates the chemical will be immobile in soil (REACH).

Calculations with a standard multimedia partitioning (fugacity) model, assuming equal and continuous distributions to air, water and soil compartments (Level III approach), predict that acetyl cedrene will be found primarily in the soil compartment (47.4%) and the water compartment (36.1%) (US EPA 2017).

Acetyl cedrene is expected to be emitted to the water and soil compartments from STP effluents and biosolids because of its use. Fugacity calculations (Level III approach) assuming sole release to the water compartment estimate the chemical will predominantly be found in the water compartment (68.7%) and sediment compartment (31.2%). With sole release to the soil compartment, the chemical is predicted to remain in soil (99.9%) (US EPA 2017).

Methyl cedryl ketone is a non-stereospecific version of acetyl cedrene. The partitioning behaviour of methyl cedryl ketone is not expected to significantly differ from acetyl cedrene.

Degradation

The chemicals in this evaluation do not degrade rapidly in the water compartment but are not persistent in air.

Acetyl cedrene will rapidly degrade by hydroxyl radicals in the atmosphere, with an estimated half-life of 1.8 hours (Aschmann et al. 2001), consistent with the calculated half-life of 1.2 hours (US EPA 2017). In addition, this chemical is highly volatile from water, with a

calculated volatilisation half-life from lake waters of 6 days (US EPA 2017). Volatilisation of acetyl cedrene to the atmosphere followed by degradation through reaction with hydroxyl radicals may, therefore, be a significant dissipation pathway in the environment.

The chemicals in this evaluation lack hydrolysable functional groups and are not expected to degrade by hydrolysis in the water compartment.

It is unclear if acetyl cedrene undergoes ultimate biodegradation in the water compartment. Acetyl cedrene is not readily biodegradable based on a study conducted in accordance with the OECD TG 301F, with 36% biodegradation by biological oxygen demand (BOD) measured over the first 21 days of the test (REACH). No further degradation was measured between day 21 and day 28 of the test, suggesting that persistent degradants were formed. No biodegradation was observed in another study conducted according to OECD TG 301C (NITE 2020).

A surface water biodegradation simulation test was conducted with acetyl cedrene according to OECD TG 309 (REACH). While test material concentrations in the water phase declined significantly over the 61 day duration of the test, only 0.7% mineralisation was observed, along with other intermediate degradation products. Two degradation products were tentatively identified: a dihydroxylated form of acetyl cedrene ($C_{17}H_{28}O_3$) and a dioxygenated form of acetyl cedrene ($C_{17}H_{26}O_3$), alongside minor polar and unidentified metabolites. Substantial amounts of the test material were recovered from the test vessel adaptor head, suggesting that the primary loss of test material from the test solution was due to volatilisation.

The environmental characteristics of the degradants of acetyl cedrene are unknown due to the lack of data. If information becomes available indicating these degradants have hazardous characteristics, the categorisation of acetyl cedrene may also change.

No studies on the degradation of methyl cedryl ketone have been identified. The chemical is anticipated to not degrade rapidly in the water compartment due to structural similarity to acetyl cedrene.

Bioaccumulation

Acetyl cedrene and methyl cedryl ketone have moderate potential to bioaccumulate in aquatic life.

The measured octanol-water partition coefficient for acetyl cedrene is above the categorisation threshold for bioaccumulation hazards in aquatic organisms (log K_{OW} ≥4.2), indicating potential for bioaccumulation (EPHC 2009).

A study conducted according to OECD TG 305 using the technical mixture of acetyl cedrene found a bioconcentration factor (BCF) value of 200–820 litres per kilogram (L/kg) wet weight (wwt) in *Cyprinus carpio* (common carp) (NITE 2020).

Another study conducted under the same test guidelines using radiolabelled acetyl cedrene gave a BCF value for the edible parts (867 L/kg wwt), head (1159 L/kg wwt) and intestines (3920 L/kg wwt) of *Oncorhynchus mykiss* (rainbow trout) (REACH). These measured values could not be converted to a whole-body lipid-normalised BCF due to the absence of fish and tissue lipid concentrations. As a result, these BCF values could not be used to assess the bioaccumulation potential of the chemical against the domestic categorisation threshold. However, they show at least moderate bioaccumulation potential for acetyl cedrene.

Therefore, acetyl cedrene is not bioaccumulative as the whole-body BCF (820 L/kg wwt) is below the domestic categorisation threshold for bioaccumulation (BCF ≥2000 L/Kg) (EPHC 2009).

No measured BCF values are available for methyl cedryl ketone. The chemical is expected have similar bioaccumulation potential to acetyl cedrene.

Environmental transport

The chemicals in this evaluation are not expected to undergo long range transport based on their short calculated half lives in the atmosphere.

Predicted environmental concentration (PEC)

The typical concentration of acetyl cedrene in Australian river water is estimated to be 1.36 µg/L, based on international monitoring data, with a reasonable worst-case concentration of 3.06 µg/L. The reasonable worst-case concentration of acetyl cedrene in domestic soil is predicted to be 0.16 milligrams per kilogram (mg/kg) dry weight (dw). These values were determined by considering available international monitoring data for acetyl cedrene in wastewater effluents, biosolids, surface water and biota. No environmental monitoring data for methyl cedryl ketone were identified and a PEC has not been determined.

Acetyl cedrene has been detected in international STP influents and effluents. Influent concentrations have been measured in the range of 0.37–13.9 µg/L (Klaschka et al. 2013; Mitjans and Ventura 2005; Simonich et al. 2000; Terzić et al. 2008). Effluent concentrations vary depending on the level of treatment, with a concentration of 3.06 µg/L measured following primary treatment (Simonich et al. 2000) and concentrations of 0.071–1.36 µg/L measured after secondary treatment (Klaschka et al. 2013; Simonich et al. 2000; Simonich et al. 2002).

The value of 1.36 µg/L in effluent after secondary treatment is taken as the estimated surface water concentration in Australia. The concentration of 3.06 µg/L in effluent after primary treatment is taken to be upper limit of surface water concentrations in Australia for the purpose of risk characterisation.

An international study detected acetyl cedrene in the surface water of rivers in Germany and Spain at concentrations of 0.016 and 0.072 µg/L, respectively (Mitjans and Ventura 2005). The chemical has also been detected in German surface waters downstream from STPs at a concentration of <0.010 µg/L (Klaschka et al. 2013).

Measured concentrations of acetyl cedrene in two sludges from international sources were 9 and 31.3 mg/kg dw (DiFrancesco et al. 2004). A literature review of biosolids contaminants found that the mean and median concentrations of acetyl cedrene in sludge from international sources were both 20.2 mg/kg dw (Langdon et al. 2010).

The calculated concentration of acetyl cedrene in soil amended with biosolids is 0.16 mg/kg dw based on mean measured international biosolid concentrations (20.2 mg/kg dw), typical biosolids application rates and a soil bulk density of 1300 kilograms per cubic metre (kg/m^3) (EPHC 2009; Langdon et al. 2010). A worst-case concentration of 0.96 mg/kg dw was calculated using the maximum measured concentration of acetyl cedrene in biosolids (31.3 mg/kg dw) and maximum biosolids application rates.

International studies have identified acetyl cedrene in aquatic biota. The chemical has been found in pike (<10–93 (µg/kg) wet weight (wwt)), eel (<10 µg/kg wwt) and barb (<10 µg/kg wwt) (Klaschka et al. 2013).

Environmental concentrations of methyl cedryl ketone have not been estimated. Based on available information, methyl cedryl ketone does not have widespread industrial use. If methyl cedryl ketone is used as a fragrance ingredient domestically it is expected to be used in small volumes compared to acetyl cedrene.

Environmental effects

Effects on aquatic Life

Acetyl cedrene and methyl cedryl ketone are expected to cause toxic effects at low concentrations in aquatic organisms across multiple trophic levels.

No experimental data for the ecotoxicity of methyl cedryl ketone were identified. The ecotoxicity data presented below for acetyl cedrene is expected to be suitable for read-across to methyl cedryl ketone given the structural similarity of the two chemicals.

Acute toxicity

The following measured median effective concentration (EC50) and median lethal concentration (LC50) values for freshwater model organisms across three trophic levels were retrieved from the REACH dossier for acetyl cedrene (REACH):

Taxon	Endpoint	Method
Fish	96h LC50 = 2.3 mg/L	*Pimephales promelas* (fathead minnow) OECD TG 203 Static conditions
Invertebrate	48h EC50 = 0.86 mg/L	*Daphnia magna* (water flea) OECD TG 202 Mobility Static conditions
Algae	96h EC50 = 4.3 mg/L	*Pseudokirchneriella subcapitata* (microalgae) OECD TG 201 Growth Static conditions

Chronic toxicity

The following measured no observed effect concentration (NOEC) values for freshwater model organisms across two trophic levels were retrieved from the REACH dossier for acetyl cedrene (REACH):

Taxon	Endpoint	Method
Invertebrates	21d NOEC = 0.087 mg/L	Daphnia magna (water flea) OECD TG 211 Reproduction Flow-through conditions
Algae	96h NOEC = 1.07 mg/L	*Pseudokirchneriella subcapitata* (microalgae) OECD TG 201 Growth Static conditions

Effects on sediment dwelling life

Two non-standard sediment ecotoxicity studies with *Capitella teleta* are available. In the first, sediment spiked with acetyl cedrene at a measured concentration of 36 mg/kg dw slightly reduced the survival rate of *Capitella teleta* over 16 days compared to the control (Ellegaard-Petersen et al. 2010). In the second, no significant effects were seen after 14 days when acetyl cedrene was spiked into sediment at measured concentrations of 34, 78, and 81 mg/kg dw (Dai et al. 2012).

Both studies identified a significant concentration loss of acetyl cedrene in the spiked sediments over the test period which may lead to an underestimation of toxicity to soil and sediment dwelling organisms.

Effects on terrestrial life

Acetyl cedrene is expected to have low acute toxicity to rats and mice through ingestion, and low acute dermal toxicity. Further information on the effects of the chemical on terrestrial organisms can be found in the acetyl cedrene Human Health AICIS Evaluation Statement (AICIS 2021).

Predicted no-effect concentration (PNEC)

The freshwater aquatic PNEC for acetyl cedrene is 8.7 µg/L.

A PNEC of 8.7 µg/L was derived from the measured invertebrate chronic ecotoxicity endpoint (21 day NOEC = 0.087 mg/L), using an assessment factor of 10. This assessment factor was selected as reliable acute and chronic ecotoxicity data are available for the most sensitive trophic level (EPHC 2009).

Categorisation of environmental hazard

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

Persistence

Persistent (P). The chemicals in this evaluation are conservatively categorised as persistent based on a water degradation half-life that may exceed the domestic categorisation threshold of 60 days.

Bioaccumulation

Not Bioaccumulative (Not B). Based on measured bioconcentration factors (BCF) for acetyl cedrene in fish that do not exceed the domestic categorisation threshold, the chemicals are categorised as Not Bioaccumulative.

Toxicity

Toxic (T). Based on available ecotoxicity values below 1 mg/L and evidence of high chronic toxicity (ecotoxicity below 0.1 mg/L) for acetyl cedrene, the chemicals are categorised as Toxic.

GHS classification of environmental hazard

Based on the available data, acetyl cedrene is classified as Acute Aquatic Category 1 (H400) and Chronic Aquatic Category 1 (H410) under the Globally Harmonised System of Classification and Labelling of Chemicals (GHS) (UNECE 2017).

Acetyl cedrene does not rapidly degrade; therefore, it meets the classification for Chronic Aquatic Category 1 from the chronic invertebrate endpoint (≤0.1 mg/L).

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
1.36	8.7	0.16

An RQ less than 1 indicates that acetyl cedrene is not expected to pose a high risk to the environment based on estimated emissions, as environmental concentrations are below levels likely to cause harmful effects. The RQ considering the worst-case PEC of 3.06 µg/L is 0.35, indicating that acetyl cedrene is not expected to pose a high risk to the environment even at worst-case concentrations in the freshwater aquatic compartment.

An RQ for acetyl cedrene in soil and sediment was not determined due to insufficient ecotoxicity and exposure data for soil and sediment dwelling organisms. Further evaluation may be required if new data become available to indicate that acetyl cedrene is present in the soil or sediment compartments at concentrations above the level of concern.

Methyl cedryl ketone is expected to have similar hazard characteristics, but much lower environmental exposures, compared with acetyl cedrene. Therefore, methyl cedryl ketone is not expected to pose a high risk to the environment.

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 no domestic monitoring data for acetyl cedrene. The measured international concentrations indicate that acetyl cedrene is present at concentrations below the level of concern. The risk profile of acetyl cedrene may change should domestic monitoring data become available to indicate that acetyl cedrene is present in Australia above the levels of concern.
- There are minimal ecotoxicity data on soil and sediment dwelling organisms available for acetyl cedrene. The risk profile of acetyl cedrene may change should new ecotoxicity data or exposure data become available to indicate that acetyl cedrene is present in Australian soil and sediment above levels of concern.
- The identity, environmental fate, and effects of the degradants of acetyl cedrene are unknown. There is evidence to suggest that acetyl cedrene does not fully mineralise, and that the degradants may be more persistent than the parent chemical. If more information becomes available in the future to indicate that these degradants may have persistent, bioaccumulative and toxic (PBT) characteristics, the PBT categorisation of acetyl cedrene may change.
- This evaluation focuses on acetyl cedrene; however, acetyl cedrene is used as a technical mixture containing impurities up to 35%. Many of the physical and chemical properties and other hazard properties were measured using the technical mixture rather than pure acetyl cedrene. It is uncertain how the impurities would impact the results of measured outcomes, though it is assumed that the properties of the structural isomers are closely modelled by acetyl cedrene. The risk profile of acetyl cedrene may change if information becomes available to indicate that the impurities in the technical mixture have more hazardous properties than acetyl cedrene.

References

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