Australian Government
Department of Health
Australian Industrial Chemicals Introduction Scheme

delta-Damascones

Evaluation statement

30 June 2022

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AICIS evaluation statement

Subject of the evaluation

delta-Damascones.

Chemicals in this evaluation

Name	CAS registry number
2-Buten-1-one, 1-(2,6,6-trimethyl-3-cyclohexen-1-yl)-	57378-68-4
2-Buten-1-one, 1-(2,6,6-trimethyl-3-cyclohexen-1-yl)-, [1.alpha.(E),2.beta.]-	71048-82-3

Reason for the evaluation

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

Parameters of evaluation

The chemicals δ-damascone (CAS RN 57378-68-4) and *trans*-rose ketone-3 (CAS RN 71048-82-3) have been assessed for risks to the environment according to the following parameters:

- Australian introduction volumes based on upper estimates provided by industry sources.
- Industrial uses listed below in the 'Summary of Use' section.
- Expected emission into sewage treatment plants (STP) due to consumer and commercial use.

These chemicals have been assessed as a group as they are structurally very similar and share the same use patterns.

Summary of evaluation

Summary of introduction, use and end use

Based on international use information, the chemicals in this group are used as fragrances in:

- Air freshener products
- Cleaning and furniture care products
- Laundry and dishwashing products
- Personal care products.

There is no information available on the domestic use volumes of these substances. Data from international jurisdictions indicate that that *trans*-rose ketone-3 is used in the European Union (EU) at 100–1000 tonnes annually, and that δ-damascone is used in the USA at up to 454 tonnes (1 000 000 lb) annually. Information provided by the International Fragrances Association (IFRA) indicated that the introduction volumes by its member companies in the Asia Pacific region (APAC) were approximately 200 tonnes of δ-damascone annually, and up to 10 tonnes of *trans*-rose ketone-3 annually. Further consultation with IFRA indicated that up to 5% of the APAC volume may be introduced for use in Australia.

Environment

Summary of environmental hazard characteristics

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

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

Environmental hazard classification

Based on the available data the chemicals are classified under the Globally Harmonised System of Classification and Labelling of Chemicals (GHS) (UNECE 2017). This evaluation does not consider classification of physical hazards and health hazards.

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 chemicals, δ-damascone and *trans*-rose ketone-3, are fragrance chemicals expected to have industrial uses in Australia. These chemicals may be released to the aquatic environment in STP effluent as a result of their uses.

These chemicals are not persistent, not bioaccumulative, and have high aquatic toxicity. Exposure modelling based on information provided by IFRA found that the estimated concentrations of the chemicals in river waters are below the level of concern (RQ < 1). The industrial use of these chemicals in Australia are therefore unlikely to pose a significant risk to the environment.

Conclusions

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

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.

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 2 closely related chemicals that belong to a group of substances called the damascones, or rose ketones. These 2 chemicals have been chosen as they appear to be chemicals from the damascones group used at the highest volumes internationally. Both chemicals, δ-damascone and *trans*-rose ketone-3, are fragrance chemicals used as ingredients in a range of consumer products. Their use in these products is expected to result in release of the chemicals to wastewater as a normal part of its use pattern.

The evaluation selection analysis of δ-damascone found that it is of potential concern to the environment based on the potential for adverse effects to aquatic organisms due to emissions to surface waters in the treated effluent discharged from STP, and possible persistent and toxic characteristics of the chemical.

Chemical identity

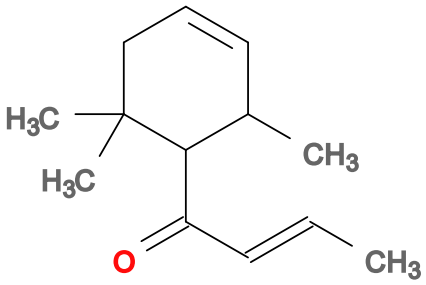
Both substances in this evaluation are members of a larger group of organic compounds known as damascones, or rose ketones. The damascones are characterised by an unsaturated cyclohexyl ring substituted on one carbon with a methyl group, on another with 2 methyl groups, and on a third, a 1,3-butenone side chain. The members of the group generally differ by the number and location of unsaturated carbon bonds in the cyclohexyl ring moiety. The 2 chemicals in this group contain an unsaturated carbon bond at the δ-position in the cyclohexyl ring.

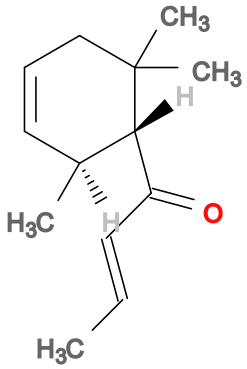
The chemical represented by CAS No. 57378-68-4 is commonly known as δ-damascone, or rose ketone-3. While its structure has 2 chiral centres, the stereochemistry of this substance is not defined in its Australian Inventory of Industrial Chemicals (AIIC) name. In addition, the geometry of its side chain alkene is not defined. Therefore, this substance is assumed to comprise a mixture of its eight stereoisomers.

The chemical represented by CAS No. 71048-82-3 is also occasionally called δ-damascone but is more commonly known as *trans*-rose ketone-3. It is a single defined stereoisomer of δ-damascone (CAS No. 57378-68-4).

Though δ-damascone and *trans*-rose ketone-3 do not occur naturally, other members of the damascones group may be found in plant extracts (Mendes et al. 2012).

CAS No.	57378-68-4
Chemical name	2-Buten-1-one, 1-(2,6,6-trimethyl-3-cyclohexen-1-yl)-
Synonyms	δ-damascone rose ketone-3 damascone delta

Structural Formula	
Molecular Formula	C13H20O
Molecular Weight (g/mol)	192.3
SMILES	C/C=C/C(=O)C1C(C=CCC1(C)C)C
Chemical description	-

CAS No.	71048-82-3
Chemical name	2-Buten-1-one, 1-(2,6,6-trimethyl-3-cyclohexen-1-yl)-, [1.alpha.(E),2.beta.]-
Synonyms	*trans*-rose ketone-3 1-(2.beta.,6,6-Trimethyl-3-cyclohexen-1.alpha.-yl)-2-butene-1-one, (E)- δ-damascone *trans-trans*-δ-damascone
Structural Formula	
Molecular Formula	$C_{13}H_{20}O$
Molecular Weight (g/mol)	192.3
SMILES	C(/C=C/C)(=O)[C@H]1C(C)(C)CC=C[C@@H]1C
Chemical description	-

Relevant physical and chemical properties

Measured and calculated physical and chemical property data for δ-damascone are presented below (REACHa; US EPA 2017). Since *trans*-rose ketone-3 is a component of δ-damascone, δ-damascone is considered a suitable read across analogue for determination of physical and chemical properties and other hazard characteristics of *trans*-rose ketone-3:

Chemical	δ-damascone
Physical form	Liquid
Melting point	10°C (exp.)
Boiling point	230°C (decomposition - exp.)
Vapour pressure	2.72 Pa at 23°C (exp.)
Water solubility	77.2 mg/L at 20°C (exp.)
Henry's law constant	15.5 $Pa \cdot m^3/mol$ (calc.)
Ionisable in the environment?	No
pKa	N/A
log K_{ow}	4.2 at 35°C (exp.)

Introduction and use

Australia

No specific Australian information on introduction, use and end use have been identified for δ-damascone or *trans*-rose ketone-3.

International

Available information indicates that δ-damascone and *trans*-rose ketone-3 are used as fragrance ingredients in a range of consumer products worldwide.

Both chemicals in this evaluation are identified as fragrance compounds on the IFRA Transparency List (IFRA), and on the European Commission Cosmetic Ingredient (CosIng) database (EC).

According to information provided by IFRA, approximately 200 tonnes of δ-damascone and less than 10 tonnes of *trans*-rose ketone-3 are introduced in the APCA-region (includes Australia) by member companies annually. Further consultation with IFRA indicated that up to 5% of the total APAC volume of δ-damascone may be introduced into Australia.

The chemical δ-damascone had a reported use volume of up to 453.6 tonnes (1 000 000 lb) in the United States in 2016 (US EPA 2016). Its uses include cleaning and furnishing care

products, laundry and dishwashing products, personal care products, air freshener products and some plastic and rubber products.

The chemical *trans*-rose ketone-3 is used in Europe in the range of 100–1000 tonnes per annum (REACHa). It is used in washing & cleaning products, biocides, air freshener products, polishes and waxes, cosmetics and personal care products and perfumes and fragrances.

The chemicals may be used in only limited concentrations in certain cosmetic types due to skin sensitisation concerns. The damascone group of chemicals is limited to a cumulative maximum concentration of 0.02% under international restrictions (see **International Regulatory status** section). Concentrations in cosmetics and household products are also restricted under the IFRA Standards (IFRA 2020).

Existing Australian regulatory controls

Environment

The industrial use of δ-damascone and *trans*-rose ketone 3 is not subject to any specific national environmental regulations.

International regulatory status

United Nations

The chemicals in this evaluation 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

Both δ-damascone and *trans*-rose ketone 3 are listed on Annex III of the EU cosmetic ingredients database (CosIng), restricting their use to a maximum concentration of 0.02% in combination with other damascone group chemicals in finished cosmetic products (EC).

New Zealand

Both δ-damascone and *trans*-rose ketone 3 are listed in New Zealand Cosmetic Products Group Standard—Schedule 5 restricting their use to a maximum concentration of 0.02% in combination with other damascone group chemicals in finished cosmetic products.

Environmental exposure

Available international use data indicate that δ-damascone and *trans*-rose ketone-3 are used as fragrances, which are incorporated into a range of product types. The formulations of such products on the Australian market are assumed to not differ significantly from those found internationally. Therefore, both chemicals may be found in a range of products available for use in Australia. This may include personal care products including perfumes, cosmetics, deodorants, automotive care products and domestic and industrial cleaners.

Chemicals used as fragrances are typically released to sewer as a normal part of their domestic applications. During treatment in STPs, chemicals may degrade by abiotic and/or biological processes, volatilise to the air compartment, partition to sludge, or remain in effluent (Struijs 1996). Depending on removal efficiencies for individual substances in sewage treatment plants, some fraction of the quantity of chemicals in wastewater entering STPs can be emitted to the air compartment, to soil through application of biosolids to agricultural land, or to rivers or oceans in treated effluent. Once released to the environment, chemicals in this group are expected to partition to the air, soil, sediment and water compartments, depending on their individual partitioning properties.

Environmental Fate

Partitioning

The chemicals in this evaluation are expected to partition to air, water and soil when released into the environment.

The chemical δ-damascone is a volatile neutral organic chemical with moderate water solubility. The calculated Henry's law constant is 15.5 Pa m^3/mol, indicating the chemical is highly volatile from water and moist soil. It is lipophilic and will adsorb to the organic component of soil. The estimated soil adsorption coefficient (K_{oc}) is 1259 L/kg based on a test in accordance with OECD Test Guideline (TG) 121 (REACHa), which indicates it has low mobility in soil.

Calculations with a standard multimedia partitioning (fugacity) model, assuming equal and continuous distributions to air, water and soil compartments (Level III output), predict that δ-damascone will partition to the soil compartment (84%) and the water compartment (16%) (US EPA 2017). With sole release into the water compartment, the chemical will predominantly remain in the water compartment (96%).

Degradation

Chemicals in this evaluation are not persistent. They degrade rapidly in air and are expected to be at least inherently biodegradable.

According to a test conducted in accordance with OECD TG 111, *trans*-rose ketone-3 has a long hydrolysis half life of 332 days (REACHa). Therefore, hydrolysis is not expected to be a major dissipation pathway in the environment.

According to calculated values δ-damascone will undergo rapid photo-oxidation by hydroxyl radicals in the atmosphere with a half life of 1.1 hours (US EPA 2017). In addition, this chemical is highly volatile from water, with a calculated volatilisation half life from lake waters of 11 days. Volatilisation of δ-damascone to the atmosphere followed by degradation through reaction with hydroxyl radicals may; therefore, be a significant dissipation pathway in the environment.

In a biodegradation screening test according to OECD TG 301C (MITI), 0% biodegradation was observed for δ-damascone over 28 days by biological oxygen demand (BOD) (REACHa). The ready biodegradability threshold of 60% by BOD was not reached.

Biodegradability standard screening tests have been conducted on related chemicals from the damascones group, including α-damascone (CAS No. 24720-09-0) and β-damascenone (CAS No. 23726-93-4). The chemical α-damascone is a structural isomer of δ-damascone,

while β-damascenone contains an additional carbon-carbon double bond in the cyclohexyl ring. These chemicals are both considered suitable analogues for read across to δ-damascone and *trans*-rose ketone-3 based on their close structural similarity.

The chemical α-damascone also failed a ready biodegradability test conducted according to OECD TG 301 C (MITI), with only 1% degradation recorded (REACHb). However, a second test conducted according to OECD TG 301 F (Manometric respirometry) resulted in 56% degradation over 28 days, and 74% degradation after extension of the test duration to 70 days. Therefore, this analogue chemical is considered inherently and ultimately biodegradable.

A ready biodegradability test conducted according to OECD 301 F (Manometric respirometry) on β-damascenone resulted in 65% degradation over 28 days, passing the biodegradation threshold of 60% but failing the 10-day window test (REACHc). Extension of the test to 48 days resulted in 77% degradation. Therefore, β-damascenone is considered inherently and ultimately biodegradable.

Therefore, chemicals δ-damascone and *trans*-rose ketone-3 are at least inherently and ultimately biodegradable, with expected biodegradation half lives below the threshold for persistence based on read across standard biodegradability results for their close analogues, α-damascone and β-damascenone.

Bioaccumulation

The chemical group in this evaluation has low potential to bioaccumulate in aquatic life.

A test conducted using δ-damascone with *Cyprinus carpio* (carp) according to OECD TG 305 found bioconcentration factors (BCF) in the range of 27–318 L/kg (REACHa). These values are below the domestic categorisation threshold for bioaccumulation (BCF ≥ 2000 L/kg) (EPHC 2009).

Environmental transport

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

Predicted environmental concentration (PEC)

The chemicals δ-damascone and *trans*-rose ketone-3 are each predicted to be present in the Australian environment at concentrations of 2.54 micrograms per litre (µg/L) in inland surface waters, and 0.35 milligrams per kilogram (mg/kg) in agricultural soil based on industry provided introduction volumes and standard sewage treatment plant process modelling. No measured concentrations of δ-damascone or *trans*-rose ketone-3 in surface waters or STP effluents were found.

Information provided by IFRA indicated up to 10 tonnes of *trans*-rose ketone-3 and approximately 200 tonnes δ-damascone are used annually in the APAC region, and that up to 5% of the volume of δ-damascone (approximately 10 tonnes) may be introduced into Australia. Therefore, introduction volumes of 10 tonnes for each chemical have been used as the Australian introduction volumes in standard exposure modelling for the release of these chemicals to surface waters in STP effluents (EPHC 2009; Struijs 1996). This modelling indicated that removal rates during STP treatment include 8% loss to volatilisation, 31% loss

through biodegradation (inherent), 19% partitioning to sludge, with the remaining 42% released in effluent for both chemicals.

The calculated concentrations of both δ-damascone and *trans*-rose ketone-3 released in effluent were 2.54 µg/L each. Considering that river flows can consist entirely of STP effluent in some drier parts of Australia, reasonable worst case environmental concentrations for δ-damascone and *trans*-rose ketone-3 in domestic rivers is predicted to be 2.54 µg/L, assuming the chemicals are released into sewers on all 365 days of the year.

The calculated concentrations of each chemical in soil amended with biosolids is 0.35 mg/kg dw based on the calculated concentrations in biosolids of 11.5 mg/kg dw, typical biosolids application rates (EPHC 2009), and a soil bulk density of 1300 kilograms per cubic metre (Langdon et al. 2010).

Environmental effects

Effects on the atmosphere

The chemicals in this group are toxic to very toxic to aquatic organisms. No measured ecotoxicity endpoints were available for *trans*-rose ketone-3. The measured endpoints for δ-damascone presented are expected to be representative of the toxicity of *trans*-rose ketone-3.

Effects on Aquatic Life

Acute toxicity

The following measured median effective concentration (EC50) and median lethal concentration (LC50) values for freshwater model organisms from 2 trophic levels for δ-damascone were retrieved from the REACH registration dossier (REACHa):

Taxon	Endpoint	Method
Fish	96 h LC50 = 0.97 mg/L	*Oryzias latipes* (medaka) OECD TG 203 Semi-static
Algae	72 h EC50 = 2.47 mg/L	*Pseudokirchneriella subcapitata* (green algae) OECD TG 201 Static

An invertebrate 48h EC50 value of 1.48 mg/L was calculated for δ-damascone and *trans*-rose ketone-3 using standard quantitative structure activity relationships (QSAR) from Ecological Structure Activity Relationships (ECOSAR) Predictive Model version 2.0 (US EPA 2020). This value was calculated from the vinyl/allyl/propargyl ketones class in ECOSAR.

Chronic toxicity

The following measured no observed effect concentration (NOEC) values for freshwater model organisms from 2 trophic levels for δ-damascone were retrieved from the REACH registration dossier (REACHa):

Taxon	Endpoint	Method
Invertebrates	21 d NOEC = 0.35 mg/L	*Daphnia magna (*water flea*)* OECD TG 211 Semi-static
Algae	72 h NOEC = 0.38 mg/L	*Pseudokirchneriella subcapitata* (green algae) OECD TG 201 Static

Effects on terrestrial Life

The chemicals in this evaluation are expected to have low to moderate acute toxicity to rats and mice through ingestion, and low acute dermal toxicity. Further information on the effects of the chemicals on terrestrial organisms can be found in the damascones Human Health IMAP tier II assessment (NICNAS 2018).

Effects on sediment dwelling life

Toxicity data for sediment swelling organisms are not available.

Predicted no-effect concentration (PNEC)

The PNEC for both δ-damascone and *trans*-rose ketone-3 is 7 µg/L.

Acute toxicity data are available for fish and algae, while chronic toxicity data are available for invertebrates and algae. Acute or chronic toxicity data are therefore, available for δ-damascone over 3 trophic levels. PNECs derived from both acute and chronic endpoints were compared and the lowest value used (EPHC 2009).

A PNEC of 9.7 µg/L was derived from the measured acute fish ecotoxicity endpoint (96 h LC50 = 0.97 mg/L) using an assessment factor of 100. This assessment factor was selected as reliable acute or chronic ecotoxicity data are available over 3 trophic levels.

A PNEC of 7 µg/L was derived from the measured chronic invertebrate endpoint (21 d NOEC = 0.35 mg/L) using an assessment factor of 50. This assessment factor was selected as reliable chronic ecotoxicity data are available over 2 trophic levels.

Categorisation of environmental hazard

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

Persistence

Not Persistent (Not P). Based on calculated rapid degradation by reaction with hydroxyl radicals in the atmosphere and evidence of inherent biodegradability based on read-across from a suitable analogue chemical, δ-damascone and *trans*-rose ketone-3 are categorised as Not Persistent.

Bioaccumulation

Not Bioaccumulative (Not B). Based on low measured BCF in fish, δ-damascone and *trans*-rose ketone-3 are categorised as Not Bioaccumulative.

Toxicity

Toxic (T). Based on available ecotoxicity values below 1 mg/L, δ-damascone and *trans*-rose ketone-3 are categorised as Toxic.

GHS classification of environmental hazard

Based on the available data δ-damascone and *trans*-rose ketone-3 are 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).

The chemical δ-damascone is not rapidly degraded and-chronic aquatic toxicity data are not available for all 3 trophic levels. Hence, according to the GHS guidance on classification of aquatic hazards, the chronic aquatic hazard of this chemical may be classified by comparing the classification based on the available chronic ecotoxicity endpoints with a classification based on the acute ecotoxicity endpoints according to the most stringent outcome method. In this case, the long term aquatic hazard of δ-damascone was classified based on the acute fish ecotoxicity endpoint.

Environmental risk characterisation

The chemicals δ-damascone and *trans*-rose ketone-3 are not persistent, not bioaccumulative, and toxic. The risk quotients (RQ = PEC ÷ PNEC) below for the riverine compartment have been calculated based on the PEC and PNEC values determined for δ-damascone and *trans*-rose ketone-3:

Chemical	PEC (µg/L)	PNEC (µg/L)	RQ
δ-damascone	2.54	7	0.36
trans-rose ketone-3	2.54	7	0. 36

The RQ value for each chemical is less than 1. This indicates that environmental concentrations of these chemicals are not expected to pose a significant risk to the environment based on the estimated emissions, as environmental concentrations are below levels likely to cause harmful effects.

As *trans*-rose ketone-3 is a component of δ-damascone, it may be appropriate to combine the introduction volumes and therefore, the RQs for these 2 chemicals. This would result in a cumulative RQ of 0.72 for these 2 chemicals, indicating cumulative concentrations are likely to be below the level of concern.

Insufficient ecotoxicity data are available to characterise the risks posed by release of these chemicals to the soil compartment. However, the chemicals are not expected to persist and

accumulate in soil based on their inherent biodegradability and expected rapid volatilisation from soil.

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 discussed below:

- There are no domestic monitoring data for the chemicals δ-damascone and *trans*-rose ketone-3. Modelled environmental concentrations of the chemicals indicate that the chemicals are present in Australia at concentrations below the level of concern. The risk profiles of δ-damascone and *trans*-rose ketone-3 may change should new Australian use volume or monitoring data become available to indicate that these chemicals may be present in Australian surface waters, sediments, or soils at concentrations above the levels of concern.
- There are minimal ecotoxicity data on soil and sediment dwelling organisms available for the chemicals in this evaluation. The risk profiles of these chemicals may change should new ecotoxicity data or exposure data become available to indicate that they may be present in Australian soil and sediment above levels of concern.

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