Australian Government
Department of Health and Aged Care
Australian Industrial Chemicals Introduction Scheme

1-Decen-4-yne

Assessment statement

27 September 2022

Final

Table of contents

AICIS assessment statement

Chemical in this assessment

Name	CAS registry number
1-Decen-4-yne	24948-66-1

Reason for the assessment

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

Certificate Application Type

Very low to low risk

Based on introduction, use and end use information described in the application, the exposure band of the introduction is 3 for human health [table item 4, clause 1] and 2 for the environment [table item 2 clause 3] of Schedule 1 *Industrial Chemicals (General) Rules 2019* (the Rules)]. The assessed chemical does not have any of the hazard characteristics in human health hazard band C (Schedule 1, clause 2) and environment hazard band D (Schedule 1, clause 4). In accordance with table item 10 section 28 and table item 12 section 29 of the Rules, the indicative human health and environment risk for the proposed introduction are both in the low risk category.

Defined scope of assessment

The chemical has been assessed:

- as imported at less than or equal to 0.1 tonne per annum; and
  - in a liquid formulation at less than or equal to 10% concentration; or
  - as a fragrance component in finished consumer products
    - at less than or equal to 1% concentration in continuous action air fresheners; or
    - at less than or equal to 0.2% concentration in fine fragrances, cosmetics, or other household products.

Summary of assessment

Summary of introduction, use and end use

The assessed chemical will be imported into Australia either in a liquid formulation at up to 10% concentration for reformulation into end use cosmetic and household products, or as a component in formulated end use cosmetic and household products. The imported or reformulated end use products will contain the assessed chemical at up to 1% concentration in continuous action air fresheners or 0.2% concentration in fine fragrances, cosmetics and other household products.

The assessed chemical in a liquid formulation at up to 10% concentration will be imported and distributed in tightly closed lacquered drums of up to 180 kg in size. Finished consumer products containing the assessed chemical at various concentrations will be packaged in containers suitable for retail sale.

Human health

Summary of health hazards

Based on the available data the assessed chemical in neat form is likely to be harmful if swallowed, a weak skin sensitiser and cause drowsiness or dizziness after a single inhalation exposure (see **Supporting information**) warranting hazard classification (see **Recommendations** section).

The available toxicity data indicate that the assessed chemical:

- is slightly irritating to skin and eyes; and
- is not genotoxic.

No data were provided for repeated dose toxicity of the assessed chemical. The assessed chemical is an olefin (alkene) with 10 carbons and has a terminal double bond and an internal triple bond. Based on the repeated dose toxicity data on alpha olefins (OECD 2001) and internal olefins (OECD 2004), the assessed chemical is not expected to cause adverse health effects from repeated exposure at low concentrations.

Hazard classifications relevant to worker health and safety

The chemical satisfies the criteria for classification according to the *Globally Harmonised System of Classification and Labelling of Chemicals* (GHS) (United Nations 2017) for hazard classes relevant for worker health and safety as follows. This does not consider classification of environmental hazards.

Health hazards	Hazard category	Hazard statement
Acute toxicity – oral	Acute Tox. 4	H302: Harmful if swallowed
Skin sensitisation	Skin Sens. 1B	H317: May cause an allergic skin reaction
Specific target organ toxicity (single exposure)	STOT Single Exp. 3	H336: May cause drowsiness or dizziness

Physical hazards	Hazard category	Hazard statement
Flammable liquids	Flam. Liquid 3	H226: Flammable liquid and vapour

Summary of health risk

Public

When introduced and used in the proposed manner, there will be widespread and repeated exposure of the public to the assessed chemical at up to 0.2% concentration through the use of a wide range of cosmetic and household products containing the assessed chemical.

The principal route of exposure will be dermal, while ocular and inhalation exposures are also possible, particularly from air care products and from products applied by spray.

The assessed chemical in neat form is likely to be harmful if swallowed, a weak skin sensitiser and cause drowsiness or dizziness after a single exposure. However, these effects are not expected, given the proposed low use concentrations at up to 0.2% concentration in fine fragrances, cosmetics and household products (other than continuous action air fresheners). While continuous action air fresheners will contain the assessed chemical at up to 1% concentration, skin sensitisation is not expected as minimal dermal exposure is expected from this use. Drowsiness or dizziness from exposure to the assessed chemical in continuous action air fresheners is also not expected given the low concentrations in finished products (up to 1% maximum is much lower than the GHS suggested cut-off concentration triggering the same classification of a mixture). Repeated dose toxicity effects from the assessed chemical are not expected due to the low use concentration of the assessed chemical in end use products, limiting systemic availability through dermal absorption.

When introduced in accordance with the terms of the assessment certificate, the assessed chemical is not considered to pose an unreasonable risk to the public.

Workers

Workers may experience exposure to the assessed chemical at up to 10% concentration during weighing and transfer stages, blending, quality control analysis and cleaning and maintenance of equipment, particularly where manual or open processes are used. Exposure to the assessed chemical in end use products (at up to 0.2% concentration) may occur in professions where the services provided involve the application of cosmetic and personal care products to clients (e.g. hairdressers and workers in beauty salons) or the use of household products in the cleaning industry.

Based on the chemical's health hazard classifications, workers may experience health effects if exposed to the assessed chemical at up to 10% concentration during formulation activities. Specific risk management measures (see **Recommendations** section) are required to manage the risks to workers.

The frequency and extent of exposure of workers applying products to clients is similar to public exposure or lower if PPE is used.

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

The assessed chemical is formally classified under the *Globally Harmonised System of Classification and Labelling of Chemicals* (GHS) (United Nations 2017) as Acute Category 1 (H400) and Chronic Category 1 (H410) based on the invertebrates toxicity data. Considerations were also made for the rapid biodegradation of the assessed chemical.

Environmental Hazard	Hazard Category	Hazard Statement
Acute Aquatic	Acute aq. – Cat. 1	H400: Very toxic to aquatic life
Chronic Aquatic	Chronic aq. – Cat 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 products. These uses may result in the release of the assessed chemical to sewers and to air.

The assessed chemical is readily degradable, not persistent and not bioaccumulative. The assessed chemical is toxic to aquatic organisms.

Although the assessed chemical is toxic, it 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 ÷ PNEC). Based on calculated 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

Recommendation to Safe Work Australia

- It is recommended that Safe Work Australia (SWA) update the *Hazardous Chemical Information System* (HCIS) to include the classification relevant to work health and safety (see **Health hazard classification**).

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 formulation activities:
    - Use of engineering controls such as
        - Enclosed and automated processes if possible
        - Adequate workplace ventilation to avoid accumulation of vapours, mists or aerosols
    - Use of safe work practices to

        - Avoid contact with skin
        - Avoid inhalation of vapours, mists or aerosols

    - Workers should wear the following personal protective equipment (PPE)
        - Protective gloves
        - Protective clothing
        - Respiratory protection where local ventilation may be inadequate

- As the assessed chemical is a skin sensitiser, employers should carry out health surveillance for any worker who has been identified in the workplace risk assessment as having a significant risk of skin sensitisation.

- The storage of the assessed chemical should be in accordance with the Safe Work Australia *Code of Practice for Managing Risks of Hazardous Chemicals in the Workplace* (SWA, 2020) or relevant State or Territory Code of Practice.

Environment

No specific recommendations for the use of the assessed chemical are required when the assessed chemical is introduced in accordance with the terms of the assessment certificate.

Conclusions

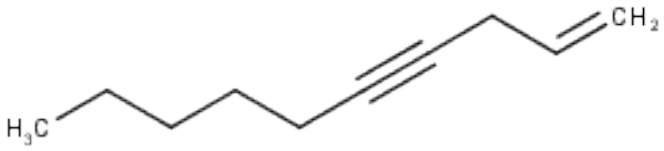
The conclusions of this assessment are based on the information described in this statement.

Considering the proposed means for managing risks, the Executive Director is satisfied that when the 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 proposed 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	1-Decen-4-yne
CAS No.	24948-66-1
Synonyms	1-Allyl-2-pentylacetylene
Structural formula	
Molecular formula	$C_{10}H_{16}$
Molecular weight (g/mol)	136.23
SMILES	C(#CCCCCC)CC=C
Chemical description	The assessed chemical has a degree of purity greater than 97%.

Relevant physical and chemical properties

Physical form	Pale yellow liquid
Melting point	< -20 °C
Boiling point	178.6 °C at 101.7 kPa
Density	787 kg/m^3 at 20 °C
Vapour pressure	91.6 Pa at 20 °C and 135 Pa at 25 °C
Water solubility	6.93 mg/L at 20 °C
Ionisable in the environment?	No
log K_{ow}	4.47
Log K_{oc}	3.84
Flash point	59.3 °C
Autoignition temperature	252 °C
Explosive properties	Not explosive

Human exposure

Workers

Reformulation

Typically, reformulation processes may incorporate blending operations that are highly automated and occur in a fully enclosed/contained environment, followed by automated filling using sealed delivery systems into containers of various sizes. Dermal, ocular and inhalation exposure (if aerosols or mists are formed) of workers to the assessed chemical at up to 10% concentration is possible during weighing and transfer stages, blending, quality control analysis, packaging and cleaning, and during maintenance of equipment. However, the exposure is expected to be minimised through the use of mechanical ventilation and/or enclosed systems, and through the use of PPE such as protective clothing and gloves, eye protection and appropriate respiratory protection.

Professional End Use

Exposure to the assessed chemical in end use products at up to 0.2% concentration may occur in professions where the services provided involve the application of cosmetic and personal care products to clients (e.g. hairdressers and workers in beauty salons) or the use of household products in the cleaning industry. These products, depending on their nature, could be applied in a number of ways, such as by hand, using an applicator or sprayed. The principal route of exposure will be dermal and inhalation (for air care products), while ocular exposure is also possible. Professionals may use PPE to minimise repeated exposure, and good hygiene practices are expected to be in place. 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 end use products containing up to 0.2% of the assessed chemical.

Public

There will be widespread and repeated exposure of the public to the chemical at up to 0.2% concentration through the use of a wide range of cosmetic and household products. The principal route of exposure will be dermal, while ocular or inhalation exposure is also possible, particularly if the products are applied by spray. Inhalation exposure is expected to be limited by the low concentrations of the assessed chemical in end use products (up to 1% in continuous action air fresheners and up to 0.2% concentration in fine fragrances, cosmetics and other household products).

Health hazard information

Acute toxicity

Oral

In an acute oral toxicity study (OECD TG 420), one rat was administered the assessed chemical at 2000 mg/kg bw in the sighting test and euthanised on Day 1 due to clinical signs of toxicity including hunched posture, pilo-erection, lethargy, body tremours, increased salivation, ataxia and splayed gait. Pale liver and pale kidneys were noted at necropsy in the animal. In the main test, there were no mortalities, clinical signs of toxicity or abnormalities at necropsy in rats administered the assessed chemical at 300 mg/kg bw (4 females).

The median lethal dose (LD50) of the chemical was determined to be greater than 300 and less than 2,000 mg/kg bw, warranting hazard classification for Acute Oral Toxicity Category 4 (H302: Harmful if swallowed) according to GHS criteria as adopted in Australia for industrial chemicals.

Inhalation

Based on an acute inhalation toxicity study (OECD TG 403), the assessed chemical in aerosol form is likely to be of low acute toxicity to rats via the inhalation route (LC50 greater than 4.9 mg/L).

There were no mortalities. Clinical signs of toxicity noted on removal from the exposure chamber included wet fur (10/10), decreased respiratory rate (10/10), body tremours (5/10), ataxia (9/10), lethargy (9/10), pilo-erection (10/10) and hunched posture (9/10). All effects were transient in nature with all animals appearing normal one day after dosing.

Abnormalities noted at necropsy included the following:
Lungs – pale, abnormally red, dark patches (10/10)
Liver – pale, patchy pallor (1/10)
Kidneys – pale (1/10)
Large intestine – gaseous distension (2/10).

The observed abnormalities were considered by the study authors to be potentially due to irritancy or local toxicity; however, this was not confirmed by histopathological examination.

Based on the results of this study, the assessed chemical meets the criteria of Specific Target organ Toxicity (STOT) Single Exposure (Category 3: Narcotic effects: H336 - May cause drowsiness or dizziness) according to GHS criteria as adopted in Australia for industrial chemicals.

Corrosion/Irritation

Skin irritation

The assessed chemical is not classified as a skin irritant, according to the results of an in vitro skin irritation test using the EpiDerm™ reconstructed human epidermis tissue model (OECD TG 439). The relative mean viability of the test substance-treated tissues was 87.6% (above the threshold for irritancy of ≤ 50%) after the 1-hour exposure period (followed by a 42-hour post-exposure incubation period).

The assessed chemical was also tested using an in vivo skin irritation test in rabbits (OECD TG 404). A single 4-hour, semi-occluded application of the test substance to the intact skin of three rabbits produced very slight to well-defined erythema and very slight to slight oedema in two animals at the 1-hour observation and the reactions persisted until the 7-day observation. Light brown discolouration of the epidermis was noted in one animal at the 24-hour, 48-hour and 72-hour observations and crust formation and/or loss of skin elasticity were noted in two animals at the 72-hour and 7-day observations. At the 14-day observation, one animal had slight desquamation and glossy skin. No corrosive effects were observed. Under the conditions of this study, the assessed chemical is a slight skin irritant but does not require classification for skin irritation according to the GHS criteria.

Eye irritation

The assessed chemical is not classified as an eye irritant, according to the results of an in vitro bovine corneal opacity and permeability (BCOP) test method (OECD TG 437). The undiluted test substance was tested through topical application to corneas for 10 minutes followed by a post-exposure incubation period of 120 minutes. The test substance resulted in a mean in vitro irritancy score (IVIS) of 2.09 (below the threshold for no classification category of ≤ 3).

The assessed chemical was also tested for eye irritation using two rabbits (OECD TG 405). A single application of the test substance produced no corneal or iridial effects. Moderate conjunctival irritation was noted in both treated eyes 1 hour after treatment and remained in one treated eye at the 24-hour observation. Minimal conjunctival irritation was observed in both treated eyes at the 48-hour observation. Treated eyes appeared normal at the 72-hour or 7-day observations. Under the conditions of this study, the assessed chemical was found to be slightly irritating to the eyes of rabbits but does not require classification for eye irritation according to the GHS criteria.

Sensitisation

Skin sensitisation

The skin sensitisation potential of the assessed chemical was assessed using a local lymph node assay (LLNA) in mice (OECD TG 429). The mice were treated by daily application of 25 µL of the test substance at concentrations of 100%, 50% or 25% (acetone/olive oil 4:1 as vehicle for 50% or 25%) to the dorsal surface of each ear for three consecutive days.

There were no deaths or signs of systemic toxicity, and body weights were comparable to controls. The stimulation index (SI) at the 100%, 50% and 25% concentrations were 7.06, 4.74 and 3.53, respectively. The concentration of test substance expected to cause a 3-fold increase in ^{3}HTdR incorporation (EC3 value) was calculated (by linear interpolation) to be 18.45%. Based on the results of this study, the assessed chemical is a weak skin sensitiser requiring hazard classification for Skin Sensitisation (Cat 1B: H317: May cause an allergic skin reaction) according to GHS criteria.

Repeated dose toxicity

No repeated dose toxicity data on the assessed chemical were provided. There are no suitable analogue data.

Genotoxicity

The assessed chemical was found to be non-mutagenic in a bacterial reverse mutation assay (OECD TG 471). The assessed chemical was also found to be non-clastogenic in an *in vitro* mammalian chromosome aberration test using human peripheral blood lymphocytes (OECD TG 473).

Environmental exposure

The assessed chemical will be imported into Australia either fully finished as a component in end-use products or in a solvent solution or as a component of liquid fragrance formulations for reformulation into end-use products. Reformulation and repackaging will occur using sealed

equipment through closed processes. Significant releases of the assessed chemical to the environment are not expected during reformulation, transport or storage.

The assessed chemical is a fragrance ingredient to be included in a range of products, resulting in a variety of potential exposure scenarios.

Use of the assessed chemical in cosmetic products, washing and cleaning 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 involve spraying of the product into the air, resulting in direct release of the assessed chemical into the air compartment.

Environmental fate

Partitioning

The assessed chemical has a high log K_{OC} value (log K_{OC} = 3.84). Therefore, the chemical is expected to partition to and become immobile in soils and sediments.

The assessed chemical is slightly water soluble (water solubility = 6.93 mg/L at 20°C). If the assessed chemical is released to surface water, a proportion of the assessed chemical is expected to remain in water compartment and a proportion of the chemical is expected to partition to sediments based on its slight water solubility and high log Koc value.

The assessed chemical is highly volatile (vapour pressure = 135 Pa at 25°C). A large proportion of the assessed chemical is expected to partition to air during STP treatment based on SimpleTreat 3.0 model outputs (Struijs, 1996). Additionally, when the assessed chemical is directly released to air it is not expected to partition to other compartments, based on the very high vapor pressure.

Degradation

Based on its measured degradation in water and predicted degradation in air, the assessed chemical is not persistent.

The half-life of the assessed chemical in air is calculated to be 2.2 hours, based on reactions with hydroxyl radicals (US EPA, 2012; calculated using AOPWIN v1.92). As its calculated half-life in air is below the domestic threshold value of 2 days, the assessed chemical is not expected to persist in the air compartment.

Degradation studies in water indicate that the assessed chemical is readily biodegradable. The result of a biodegradation study supplied for the assessed chemical was 89% degradation (OECD 301F) over 28 days and satisfied the 10-day-window criterion.

Bioaccumulation

Based on the weight of evidence, the assessed chemical is considered not bioaccumulative.

The experimental partition coefficient of the assessed chemical is log K_{OW} = 4.47, which is above the domestic bioaccumulation threshold value of log K_{OW} = 4.2. However, calculated

BCF values, using the BCFBAF v3.01 model (US EPA, 2012), for the assessed chemical are below the domestic bioaccumulation threshold of 2000 L/kg (EPHC, 2009). The assessed chemical falls within the log K_{OW} and molecular weight applicability domains of the model. As the assessed chemical also meets the criteria for being readily biodegradable, the chemical is considered to be not bioaccumulative based on the weight of evidence.

Predicted environmental concentration (PEC)

A predicted environmental concentration (PEC) for Australian waters was calculated assuming 100% of the introduction volume is released into sewage treatment plants (STPs) over 365 days per annum. This calculated value is conservative as not all uses of the assessed chemical are expected to result in 100% release to STPs. Based on its very high vapour pressure, a large proportion of the assessed chemical is expected to partition to air during STP treatment. In addition, as the assessed chemical has high log Kow and is readily biodegradable, it is expected to be removed through biodegradation and adsorption to biosolids during STP treatment. As a result, only a very small proportion of the assessed chemical is expected to be present in STP effluent. The extent to which the assessed chemical is removed from the effluent in STP processes is based on its physicochemical properties, modelled by SimpleTreat 3.0 (Struijs, 1996) and is estimated to be 96%. Therefore 4% of the total introduction volume is estimated to be released to the aquatic environment. The calculation of the PEC is detailed in the table below:

Total Annual Import Volume	10,000	kg/year
Proportion expected to be released to sewer	100 %	
Annual quantity of chemical released to sewer	10,000	kg/year
Days per year where release occurs	365	days/year
Daily chemical release	0.27	kg/day
Water use	200	L/person/day
Population of Australia	24.386	Million
Removal within STP	96 %	Mitigation
Daily effluent production	4 877	ML/day
Dilution Factor - River	1.0	
Dilution Factor - Ocean	10.0	
PEC - River	0.003	µg/L
PEC - Ocean	0.0003	µg/L

These PEC values are further considered to be conservative as a portion of the calculated assessed chemical in the effluent will partition to sediments, based on the assessed chemicals log Koc value.

Environmental effects

Effects on Aquatic Life

Acute toxicity

The following key measured median lethal concentration (LC50), effective concentration (EC50) and inhibition concentration (IC50) values for model organisms were supplied for the assessed chemical:

Taxon	Endpoint	Method
Fish	96 h LC50 = 1.21 mg/L	*Danio rerio* (zebra fish) Mortality OECD TG 203 Semi-static conditions Measured concentration
Invertebrate	48 h EC50 = 0.564 mg/L	*Daphnia magna* (water flea) Immobility OECD TG 202 Semi-static conditions Measured concentration
Algae	72 h EC50 = 1.15 mg/L	*Pseudokirchneriella subcapitata* (green algae) growth rate OECD TG 201 Semi-static conditions Measured concentration
Microorganisms	3 h IC50 = 38.7 mg/L	Activated sludge from a STP Respiration inhibition OECD TG 209 Static conditions Nominal concentration

Chronic toxicity

The following measured 10th-percentile effective concentration (EC10) value for model organisms was supplied for the assessed chemical:

Taxon	Endpoint	Method
Algae	72 h EC10 = 0.271 mg/L	*Pseudokirchneriella subcapitata* (green algae) growth rate OECD TG 201 Semi-static conditions Measured concentration

Predicted no-effect concentration (PNEC)

A predicted no-effect concentration (PNEC) of 5.64 µg/L was calculated for the assessed chemical in the aquatic environment. This value was derived using the most conservative endpoint value for invertebrates (0.564 mg/L). An assessment factor of 100 was applied to this endpoint as acute toxicity data was provided for all three trophic levels and chronic toxicity data was provided for one tropic level (EPHC, 2009). The acute endpoint was selected, over the algal chronic endpoint, in the absence of additional chronic endpoints to support the algal growth rate EC10 value (ECHA 2008).

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 (not P). Based on measured degradation during screening tests, the assessed chemical is categorised as not Persistent.

Bioaccumulation

Not bioaccumulative (not B). Based on the weight of evidence, the assessed chemical is categorised as not Bioaccumulative.

Toxicity

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

Environmental risk characterisation

Although the assessed chemical is 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.

Based on the PEC and PNEC values determined above, Risk Quotients (RQ = PEC ÷ PNEC) have been calculated for release of the assessed chemical to water:

Compartment	PEC	PNEC	RQ
River	0.003 µg/L	5.64 µg/L	< 0.01
Ocean	0.0003 µg/L	5.64 µg/L	< 0.01

For the river and ocean compartments, an RQ less than 1 indicates that the environmental risk from the assessed chemical can likely be managed based on estimated releases, as environmental concentrations are below the levels that are likely to cause harmful effects.

References

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