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

Benzene, 1-(2-methylpropyl)-4-(propoxymethyl)-

Assessment statement (CA09651)

14 February 2023

Table of contents

Contents

AICIS assessment statement

Chemical(s) in this assessment

Name	CAS registry number
Benzene, 1-(2-methylpropyl)-4-(propoxymethyl)-	1631962-93-0

Reason for the assessment

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

Certificate Application type

Health focus

According to information submitted by the applicant and criteria in the *Industrial Chemicals (General) Rules 2019* and the Industrial Chemicals Categorisation Guidelines, this introduction is in the **assessed** category. The reason is that this introduction has **medium to high** indicative risk for **human health** because it is in:

- human health exposure band 4
- human health hazard band B

The introduction of this chemical has **low** indicative risk for the **environment** because it is in:

- environment exposure band 2
- environment hazard band C

Defined scope of assessment

The chemical has been assessed:

- as a fragrance component imported into Australia at up to 1 tonne per annum
- imported as a component of liquid fragrance formulations at up to 10% concentration, for local reformulation into finished cosmetic and household products
- imported or formulated as a component of finished cosmetic and household products up to:
    - 0.03% concentration in non-spray deodorant
    - 0.1% concentration in leave-on cosmetic products
    - 0.2% concentration in fine fragrances
    - 0.4% concentration in hair care products
    - 0.6% concentration in rinse-off cosmetic and household products
    - 5% concentration in air care products

Summary of assessment

Summary of introduction, use and end use

The assessed chemical will not be manufactured in Australia. It will be imported into Australia up to 1 tonne/year at up to 10% concentration in blended fragrance oils in 250 L polypropylene-lined steel drums and transported to the applicant's Australian facilities.

Reformulation activity will not take place at the applicant's Australian facilities. The drums containing the assessed chemical will be stored at the applicant's facilities until sold to the industrial and commercial customers for further reformulation into wide range of cosmetic and household products.

Finished cosmetic and household products containing the assessed chemical will be widely used by both consumers and professionals (such as beauticians, hairdressers, and childcare workers). Depending on the nature of the product, application may be by hand or through the use of an applicator. The proposed maximum use concentrations of the assessed chemical in various cosmetics and household products will be up to 0.1% concentration in leave on cosmetic products, up to 0.6% concentration in rinse-off cosmetic and household products, up to 0.4% concentration in hair care products, up to 0.2% concentration in fine fragrances, and up to 5% concentration in air care products.

Human health

Summary of health hazards

Based on the data provided, the assessed chemical is likely to be sensitising to the skin (see **Supporting information**), warranting hazard classification (see **Health hazard classification** section).

The applicant has not provided data on inhalation toxicity.

The data provided indicate that the assessed chemical:

- is of low acute oral toxicity
- is not irritating to skin and eyes
- is not considered to be genotoxic
- is not likely to cause systemic toxicity following repeated oral exposure up to 47.8 mg/kg bw/day in rats

Hazard classifications relevant for worker health and safety

Based on the available data, the assessed chemical satisfies the criteria for classification for human health according to the *Globally Harmonised System of Classification and Labelling of Chemicals* (GHS) (UNECE 2017), as adopted for industrial chemicals in Australia.

Health hazards	Hazard category	Hazard statement
Skin Sensitisation	Skin Sens. 1B	H317 – May cause an allergic skin reaction

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 0.6% 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 or inhalation exposure is also possible, particularly from products applied by spray and also through the use of air care products.

The assessed chemical is a skin sensitiser (Category 1B). Given the maximum proposed use concentrations of the assessed chemical (at up to 0.6% concentration), skin sensitisation effects are not expected. Similarly, skin sensitisation effects are also not expected when the assessed chemical is used at up to a concentration of 5% in air care products.

The repeated dose toxicity potential of the assessed chemical was estimated by calculating the margin of exposure (MoE), with total daily systemic exposure estimated as 0.3242 mg/kg bw/day (see Human exposure section under **Supporting information**). Using a conservative no-observable-adverse-effect-level (NOAEL) of 47.8 mg/kg bw/day, which was derived from a repeated dose oral toxicity study on the assessed chemical in female rats, the MoE was estimated to be 147. A MoE value of greater than or equal to 100 is considered acceptable to account for intra- and inter-species differences.

This assessment does not identify any risks to public health that would require specific risk management measures when the assessed chemical is introduced in accordance with the terms of the assessment certificate.

Workers

Potential exposure of workers to the assessed chemical at up to 10% concentration may occur during various formulation and packaging operations. The exposure to the assessed chemical will be mainly dermal and ocular and occasional inhalation exposure.

Exposure to the assessed chemical in end use products at up to 0.6% 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.

Given that risks of critical health effects (skin sensitisation) of the assessed chemical, control measures to minimise dermal exposure are needed to manage the risk to workers (see Means for managing risk section). Control measures to minimise inhalation exposure may be also needed if aerosols or mists are formed during the blending process.

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)
- Bioaccumulative (B)
- Toxic (T)

Environmental hazard classification

The chemical satisfies the criteria for classification according to the *Globally Harmonized System of Classification and Labelling of Chemicals* (GHS) (UNECE 2017) as Acute Category 1 (H400) and Chronic Category 1 (H410) based on the toxicity data for invertebrates and algae. Considerations were also made for the rapid degradation of the assessed chemical.

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

Summary of environmental risk

The assessed chemical will be introduced as a fragrance ingredient for use in a variety of products. These uses may result in the release of the assessed chemical to sewers and to air. In these compartments, the assessed chemical is expected to partition between the air, water and sediment compartments.

The assessed chemical is readily biodegradable and is not persistent. The assessed chemical has potential to bioaccumulate and is toxic to aquatic organisms.

Although the assessed chemical is toxic and potentially bioaccumulative, it does not meet all three PBT criteria. The environmental 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

Recommendation to Safe Work Australia

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

Information relating to safe introduction and use

- The following control measures could be implemented to manage the risk arising from exposure to the assessed chemical during reformulation activities:
    - Use of engineering controls such as
        - Enclosed and automated processes where 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 mists or aerosols

    - Use of personal protective equipment (PPE)
        - Impervious gloves
        - Protective clothing
        - Respiratory protection where local ventilation may be inadequate

- 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.

- A copy of the Safety Data Sheet (SDS) should be easily accessible to workers.

Environment

Information relating to safe introduction and use

The chemical may be scheduled under the Industrial Chemicals Environmental Management (Register) Act 2021. Information from this assessment statement will be considered as part of any scheduling process. This may include information on chemical identity, environmental hazard characteristics, GHS classification and environmental risk.

Conclusions

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

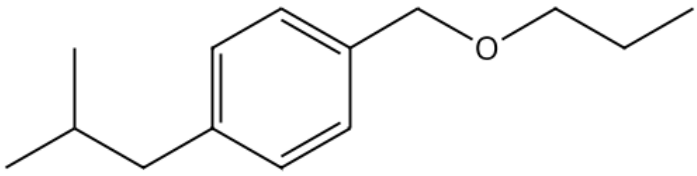
Considering the means of managing risks, the Executive Director is satisfied that when the assessed chemical is introduced and used in accordance with the terms of the assessment certificate, the human health and environment risks can be managed. This is provided that:

- all requirements are met under environmental, workplace health and safety and poisons legislation as adopted by the relevant state or territory.
- the means of managing the risks identified during this assessment are implemented.

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

Supporting information

Chemical identity

Chemical name	Benzene, 1-(2-methylpropyl)-4-(propoxymethyl)-
CAS No.	1631962-93-0
Synonyms	4-(2-Methylpropyl)benzyl propyl ether 1-(2-Methylpropyl)-4-(propoxymethyl)benzene
Molecular formula	$C_{14}H_{22}O$
Molecular weight (g/mol)	206.32
SMILES	O(CC1=CC=C(C=C1)CC(C)C)CCC
Chemical description	Small organic molecule, ether
Structural formula	

Relevant physical and chemical properties

All measured values are based on the studies provided on the assessed chemical and conducted according to OECD test guidelines.

Physical form	Colourless liquid
Melting point	< -25 °C
Boiling point	268 °C
Density	897 kg/m^3 at 20 °C
Vapour pressure	1.7 Pa at 25 °C
log K_{ow}	5.5 at 25 °C
Water solubility	3.4 mg/L at 20 °C
Surface tension	54.5 mN/m at 20 °C
Flash point	104 °C at 101.3 kPa
Auto flammability	298 °C at 101.3 kPa

Ionisable in the environment? No

Adsorption (log K_{oc}) 3.98

Human exposure

Workers

As indicated by the applicant, reformulation and packaging processes at the applicant's customers' facilities may incorporate blending operations that are highly automated to a great extent. Dermal, ocular and may be inhalation exposure (if aerosols or mists are formed) of workers to the assessed chemical at up to 10% concentration and at lower concentrations is possible during weighing and transfer stages, blending, quality control analysis, packaging into containers of various sizes, cleaning, and during maintenance of equipment.

According to the applicant, the exposure is expected to be minimised through the use of personal protective equipment (PPE) such as protective clothing, eye protection, chemical resistant gloves, and appropriate respiratory protection. In addition, the facility is expected to provide adequate local ventilation and self-contained breathing apparatus' if required. The production process will be in compliance with Good Manufacturing Practices, including the availability of eyewash stations and/or safety showers in the vicinity of the blending areas.

Public

There will be widespread and repeated exposure of the public to the assessed chemical at up to 0.6% 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 from products applied by spray and also through the use of air care products.

Data on typical use patterns of cosmetic and household cleaning product (SCCS 2012; Cadby et al. 2002; ACI 2010; Loretz et al. 2006) in which the assessed chemical may be used are shown in the following tables. For the purposes of the exposure assessment, Australian use patterns for the various product categories are assumed to be similar to those in Europe. In the absence of dermal absorption data, a dermal absorption (DA) of 100% was assumed for the assessed chemical (ECHA 2017). A lifetime average female body weight (BW) of 70 kg (enHealth 2012) was used for calculation purposes. For the inhalation exposure assessment, a 2-zone approach was used (Steiling et al. 2014; Rothe et al. 2011; Earnest Jr. 2009). An adult inhalation rate of 20 m^3/day (enHealth 2012) was used and it was conservatively assumed that the fraction of the assessed chemical inhaled is 50%.

Cosmetic products (dermal exposure)

Product type	Amount (mg/day)	C (%)	RF	Daily systemic exposure (mg/kg bw/day)
Body lotion	7820	0.100	1.000	0.1117
Face cream	1540	0.100	1.000	0.0220
Hand cream	2160	0.100	1.000	0.0309

Fine fragrances	750	0.200	1.000	0.0214
Deodorant (non-spray)	1500	0.030	1.000	0.0064
Shampoo	10460	0.600	0.010	0.0090
Conditioner	3920	0.600	0.010	0.0034
Shower gel	18670	0.600	0.010	0.0160
Hand wash soap	20000	0.600	0.010	0.0171
Hair styling products	4000	0.600	0.100	0.0343
Facial cleanser	800	0.600	0.010	0.0007
Total				**0.2729**

Daily systemic exposure = (Amount × Chemical concentration × RF × DA absorption)/BW
(RF = retention factor; DA = dermal absorption; BW = body weight)

Household products (Indirect dermal exposure – from wearing clothes):

Product type	Amount (g/use)	C (%)	Product Retained (PR) (%)	Percent Transfer (PT) (%)	Daily systemic exposure (mg/kg bw/day)
Laundry liquid	230	0.6	0.95	10	0.0187
Fabric softener	90	0.6	0.95	10	0.0073
Total					**0.0261**

Daily systemic exposure = (Amount × C × PR × PT × DA)/BW
(C = chemical concentration; PR = product retained; PT = product transferred; DA = dermal absorption; BW = body weight)

Household products (Direct dermal exposure):

Product type	Frequency (use/day)	C (%)	Contact area (cm^2)	Product usage (g/cm^3)	Film thickness (cm)	Time scale factor	Daily systemic exposure (mg/kg bw/day)
Laundry liquid	1.43	0.6	1980	0.01	0.01	0.007	0.0002
Dishwashing liquid	3	0.6	1980	0.009	0.01	0.03	0.0014
All-purpose cleaner	1	0.6	1980	1	0.01	0.007	0.0119
Total							**0.0134**

Daily systemic exposure = (Frequency × C × Contact area × Product Usage × Film Thickness × Time Scale Factor × DA)/BW
(C = chemical concentration; DA = dermal absorption; BW = body weight)

Hair spray (Inhalation exposure):

Amount (g/day)	C (%)	Inhalation rate (m^3/day)	Exposure duration (min)		Fraction inhaled (%)	Airspace volume (m^3)		Daily systemic exposure (mg/kg bw/day)
			Zone 1	Zone 2		Zone 1	Zone 2	
9.89	0.4	20	1	20	50	1	10	**0.0118**

Daily systemic exposure = [(Amount × C × 20 m^3/day Inhalation Rate × 50% Fraction Inhaled × 0.1)/BW× 1440)] × (Exposure Duration Zone 1/Volume Zone 1 + Exposure Duration Zone 2/Volume Zone 2)
(C = chemical concentration; BW = body weight)

The worst case scenario estimation using these assumptions is for a person who is a simultaneous user of all products listed in the above tables that contain the assessed chemical. This would result in a combined internal dose of 0.3242 mg/kg bw/day. It is acknowledged that inhalation exposure to the assessed chemical from use of other cosmetic and household products (in addition to hair spray) may occur. However, it is considered that the combination of the conservative (screening level) hair spray inhalation exposure assessment parameters, and the aggregate exposure from use of all dermally applied products, which assumes a conservative 100% absorption rate, is sufficiently protective to cover additional inhalation exposure to the notified chemical from use of other spray cosmetic and household products with lower exposure factors (e.g., air fresheners).

Health hazard information

Acute toxicity

Oral

In an acute oral toxicity study (OECD TG 420), the assessed chemical was administered to a group of fasted female Wistar rats (n=5) at a single dose of 2000 mg/kg bw via oral gavage. The animals were observed for 14 days after administration. All animals survived until the end of the 14-day study period and no sign of clinical toxicity was noted. All animals showed the expected body weight gains over the study period. No treatment-related gross necropsy findings were observed. The acute oral median lethal dose (LD50) of the assessed chemical was determined to be >2000 mg/kg bw.

Corrosion/Irritation

Skin irritation

The assessed chemical was determined not to be irritating to the skin in an *in vitro* skin irritation test, using the EpiSkin™ reconstructed human epidermis (RHE) (SkinEthic RHE® model) (OECD TG 439). The relative mean viability of the test chemical-treated tissues was 106.6% (considered as 100%) after the 15 minutes exposure period (followed by 42 hours post-exposure incubation period). Under the conditions of this study and according to the test guideline, the assessed chemical was not considered to be irritating to the skin.

The assessed chemical was determined not to be corrosive to the skin in an *in vitro* skin corrosivity test using the EpiDerm™ reconstructed human epidermis tissue model (EpiDerm™ tissue) (OECD TG 431). The relative mean viability of the test chemical-treated tissues was 95.4% after the 3 minutes exposure period and 99.2% after 1 hour exposure period. Under the

conditions of this study and according to the test guideline, the assessed chemical was not considered to be corrosive to the skin.

Eye irritation

The eye irritation potential of the assessed chemical was determined using Bovine Corneal Opacity and Permeability (BCOP) test method (OECD TG 437) by application of 750 µL test material (undiluted) into the anterior part of each holder containing isolated bovine cornea for 10 minutes (OECD TG 437). An *In vitro* Irritancy Score (IVIS) was calculated, with an IVIS greater than 55 being indicative of risk of serious damage to eyes. The IVIS score of the test-substance was determined to be -1.3 based on corneal opacity and permeability endpoints. Under the conditions of this study and according to the test guideline, the assessed chemical does not cause serious eye damage in the BCOP test.

Sensitisation

Skin sensitisation

One *in chemico* and two *in vitro* cell based assays were conducted to evaluate the skin sensitisation potential of the assessed chemical. These tests are part of Integrated Approach to Testing and Assessment (IATA) which address specific key events of the Adverse Outcome Pathway (AOP) leading to development of skin sensitisation (OECD, 2016) 497 (June 2021).

The direct peptide reactivity assay (DPRA) is a *chemico* method and aims to address the first key event (KE) (molecular initiation) of the AOP by measuring the interaction of the assessed chemical with cysteine and lysine, small synthetic peptides representing the nucleophilic centres in skin proteins (OECD TG 442C). The ARE-Nrf2 luciferase assay aims to address the second key event (keratinocyte activation) of the AOP by measuring the expression of a reporter luciferase gene under the control of a promoter from the antioxidant response element (ARE), a responding gene known to be upregulated by contact sensitisers (OECD TG442D). In the third key event assay, the Human Cell Line Activation test (h-CLAT) assay, the skin sensitization potential of the test substance is evaluated by measuring the changes in the expression of cell surface markers (CD54 and CD86) associated with the process of dendritic cell activation in the human leukemia cell line (THP-1) following exposure to test substance (OECD TG 442E). The results of these assays are considered using the applicable DA in the DASS Guideline for Classification and Labelling purposes. Based on the results of the AOP assays and using the DA ‘two out of 3’ in the DASS Guideline (No: 497), the assessed chemical is a skin sensitiser.

To confirm the skin sensitisation potency of the assessed chemical, the applicant has provided data from an analogue chemical using a local lymph node assay (LLNA) (OECD TG 429). Three groups of five female mice (CBA/Ca) (5 animals/dose) received topical applications (25 µL/ear) of the analogue chemical to the entire dorsum of each ear lobe at 25%, 50% and 100% (v/v) concentrations in 20% (v/v) in acetone/olive oil (4:1) for 3 consecutive days. On day 6, 250 µL (20 µCi/mouse) of ^{3}HTdR (80 µCi/mL) solution was injected via the tail vein and the animals were euthanised approximately 5 hours afterward for further processing.

There were no deaths or signs of systemic toxicity. The analogue chemical at 25%, 50% and 100% (v/v) concentrations in acetone/olive oil (4:1) (w/v) produced a Stimulation Index (SI) 4:1 of 4.32, 7.43 and 15.53, respectively. The analogue chemical was characterised as a skin sensitiser and the concentration of the analogue chemical expected to cause a 3-fold increase in 3HTdR incorporation (extrapolated EC3 value) was calculated to be 18.6%.

The skin sensitising potential of a diluted concentration of the assessed chemical was further evaluated in a human repeat insult patch test (HRIPT) (modified Shelanski human patch test method) in 108 subjects. The assessed chemical at 1% concentration solution in a mixture of ethanol and diethyl phthalate (Ethanol:DEP 25:75) was applied under occlusive patch to the upper back of each subject and was allowed to remain in direct skin contact for a period of 24 hours. Patches were applied to the same site for three alternative days for a total of 9 applications during the induction period. After a 2-week rest period, the subjects were rechallenged at a virgin site for 24 hours and the reactions were scored over a period of 3 days. No skin reactions were observed during the induction or challenge stage on any subjects. The study authors concluded that the assessed chemical at up to 1% concentration did not demonstrate a potential for eliciting skin irritation or sensitisation under the test conditions.

The positive results of the analogue chemical in the LLNA test confirmed the assessed chemical as a skin sensitiser. Using the EC3 value of the analogue chemical (18.6%) with GHS criteria for classification, the assessed chemical is determined to be a Category 1B skin sensitiser (H317: May cause an allergic skin reaction).

Repeat dose toxicity

Oral

In a repeated dose oral toxicity study (OECD TG 407), the assessed chemical was administered to Wistar rats (6/sex/dose) by oral gavage for 28 days at 300 ppm (55 and 47.8 mg/kg bw/day in males/females), 900 ppm (163 and 131.6 mg/kg bw/day in males/females) and 2700 ppm (491.4 and 418.4 mg/kg bw/day in males/females). An additional group of rats (6/sex) were fed the assessed chemical at 2700 ppm (458.9 and 410.7 mg/kg bw/day in males/females) to assess the reversibility of any effects following a 14-day recovery period.

No clinical signs of toxicity, mortality or changes in haematology and coagulation parameters, and functional observation battery tests were observed throughout the treatment and recovery period for all tested concentrations of the assessed chemical. The mean body weights, absolute and total weight gains and food consumption were lower towards the end of treatment period at 2700 ppm concentration in both sexes (mean body weights reduced by -7.1% to -7.3% in males and -7.0% to -7.5% in females). However, the terminal body weights were not affected by the treatment at any of the tested doses in either sex. With regards to organ weights, increased mean liver weight was observed at 900 ppm (11% increase in males, 14% increase in females) and at 2700 ppm (increases of 28% in males and 39% in females) of the assessed chemical.

Grossly, pale discolouration of liver was observed in both sexes at 2700 ppm and was associated with hepatocyte vacuolation/hepatocellular hypertrophy and considered as test item-related change. Increased liver weight in this group was associated with minimal hepatocellular hypertrophy with centrilobular distribution in both sexes. In addition, hepatocyte vacuolation (micro-vesicular) was also observed in males and in females at 900 and 2700 ppm. The severity of hepatocyte vacuolation was minimal to mild with periportal distribution. The hepatocytes with micro vesicular vacuolation appeared pale with foamy cytoplasmic appearance (multiple small vacuoles filled the cytoplasm without displacement of hepatocyte nuclei). At the end of 14 days recovery period, liver weight increase was completely reversible in males and partially reversible in females (6% increase reported).

Under the conditions of this study, the no-observed-adverse-effect level (NOAEL) was established as 300 ppm (55 and 47.8 mg/kg bw/day for males/female rats).

Genotoxicity

The assessed chemical was found to be non-mutagenic in a bacterial reverse mutation assay using *Salmonella typhimurium* strains TA98, TA100, TA1535, TA1537 and *Escherichia coli* strain WP2uvrA (pKM101), with or without metabolic activation (S9-mix) (OECD TG 471). No significant increases in the frequency of revertant colonies were recorded for any of the bacterial strains at any tested dose (5, 15, 50, 150, 500, 1500, 5000 µg/plate), with or without metabolic activation (S9-mix).

The assessed chemical was also found to be non-mutagenic in an *in vitro* Mammalian Chromosomal Aberration test using human lymphocytes, with or without metabolic activation (S9) (OECD TG 473). No statistically significant increases in the proportion of polyploid or endoreduplicated metaphase cells were observed after 3 hours exposure period at any tested dose, with (140, 160, 190 µg/mL) or without (20, 30, 40 µg/mL) metabolic activation (S9). The assessed chemical also showed no mutagenic properties after 21 hours exposure at any tested dose (5, 20, 22.5 µg/mL), without metabolic activation.

Environmental exposure

The assessed chemical will be introduced to Australia as a component in blended fragrance oils. No manufacture of the blended fragrance oils containing the assessed chemical will occur in Australia.

The blended fragrance oils containing the assessed chemical will be imported and stored locally in Australia until sold to industrial and/or commercial customers to be reformulated into a variety of consumer products. At the storage facility, primary work activities will include handling, loading and off-loading of drums containing finished fragrance oils formulated with the assessed chemical. Significant releases of the assessed chemical to the environment are not expected during this handling or transport process. Reformulation of products containing the assessed chemical will occur at customers' facilities and is expected to be largely automated.

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

Consumer end-uses of the assessed chemical in cosmetic products and 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.

Consumer end-use of the assessed chemical in polishes and wax blends is not expected to result in significant releases of the assessed chemical to the environment.

Consumer end-use of the assessed chemical in air care products will result in direct release of the assessed chemical into the air compartment.

Environmental fate

Partitioning

The assessed chemical is slightly water soluble (water solubility = 3.4 mg/L at 20°C), volatile (vapour pressure = 1.7 Pa at 25°C) and has a high log K_{OC} value (log K_{OC} = 3.98). When the

chemical is released to water, a considerable proportion of the chemical is expected to evaporate and partition to air. The remainder of the assessed chemical is expected to stay in water or partition to, and become immobile in, sediments.

The assessed chemical is not expected to partition out of the air compartment when released to air.

Degradation

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

Two ready biodegradation screening tests conducted using the OECD 301F test guideline were supplied for the assessed chemical. One study, using 21.3 mg/L of test substance (~63 mg/L ThO_2D), demonstrated 97.6% biodegradation by day 28 and satisfied the 10-day window. Another study, using 100 mg/L of test substance, demonstrated 1% degradation after 28 days. Both tests fulfilled the OECD TG 301F validity criteria. The difference in biodegradation between the two studies may be due to differences in test substance to inoculum ratio, or to the natural variation between different inoculum sources. The assessed chemical is considered to be readily biodegradable based on the positive result.

Although hydrolytic rate and half-lives were not quantifiable under OECD TG 111 test conditions, the supplied hydrolysis information suggests that the assessed chemical will be unstable in water under environmentally relevant conditions.

The half-life of the assessed chemical in air is calculated to be 4.9 hours, based on reactions with hydroxyl radicals (US EPA, 2012; calculated using AOPWIN v1.92). As its 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.

Bioaccumulation

The assessed chemical is potentially bioaccumulative based on its log K_{OW} value.

No bioaccumulation information was provided for the assessed chemical. The measured partition coefficient of the assessed chemical is log K_{OW} = 5.5, which exceeds the domestic bioaccumulation threshold of log K_{OW} = 4.2 (EPHC, 2009). This determination is conservative as the assessed chemical is not considered to be persistent.

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 (STP) over 365 days per annum. The extent to which the assessed substance is removed from the effluent in STP processes is based on its physicochemical properties, modelled by SimpleTreat 3.0 (Struijs, 1996).

Based on the partitioning and biodegradability of the assessed chemical, a moderate portion (19%) of the assessed chemical will undergo biodegradation while a large proportion (71%) of the assessed chemical is expected to partition to sludge. Total removal during STP treatment is estimated to be 94%. Therefore, 6% of the total introduction volume is estimated to be released to the aquatic environment.

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

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

Total Annual Import Volume	1000	kg/year
Proportion expected to be released to sewer	100 %	
Annual quantity of chemical released to sewer	1000	kg/year
Days per year where release occurs	365	days/year
Daily chemical release	2.74	kg/day
Water use	200.0	L/person/day
Population of Australia	25.423	Million
Removal within STP	94 %	Mitigation
Daily effluent production	5085	ML/day
Dilution Factor - River	1.0	
Dilution Factor - Ocean	10.0	
PEC - River	0.03	µg/L
PEC - Ocean	0.003	µg/L

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

Environmental effects

Effects on aquatic Life

Acute toxicity

The following median effective concentration (EC50) values for model organisms were supplied by the applicant:

Taxon	Endpoint	Method
Invertebrate	48 h EC50 = 0.21 mg/L	*Daphnia magna* (water flea) Immobility OECD TG 202 Semi-static conditions Measured concentration
Algae	72 h ErC50 = 0.30 mg/L	*Pseudokirchneriella subcapitata* (green algae) Growth rate OECD TG 201 Static conditions Measured concentration

Chronic toxicity

The following measured no-observed-effect concentrations (NOEC) values for model organisms were supplied by the applicant:

Taxon	Endpoint	Method
Algae	72 h NOEC = 0.095 mg/L	*Pseudokirchneriella subcapitata* (green algae) Growth rate OECD TG 201 Static conditions Measured concentration

Predicted no-effect concentration (PNEC)

A predicted no-effect concentration (PNEC) of 0.42 µg/L was calculated for the assessed chemical in the aquatic environment. This value was derived using the most conservative endpoint value for invertebrates (0.21 mg/L). An assessment factor of 500 was applied to this endpoint as acute toxicity data was available for two trophic levels and chronic toxicity data was incomplete (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 NOEC (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 test conditions, the assessed chemical is categorised as Not Persistent.

Bioaccumulation

Bioaccumulative (B). Based on high measured log K_{OW} value, indicating a potential to bioaccumulate, the assessed chemical is categorised as 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 and potentially bioaccumulative, it does not meet all three PBT criteria and 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	0.03 µg/L	0.42 µg/L	0.07
Ocean	0.003 µg/L	0.42 µg/L	<0.01

For the river and ocean compartments, an RQ less than 1 indicates that introduction of the assessed chemical, in line with the terms outlined in this assessment certificate, is not expected to pose a significant risk to the environment. As such, the risk from the assessed chemical can likely be managed, based on consideration of the environmental hazard characteristics and estimated releases.

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