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

# 1-Propanaminium, *N*,*N*,*N*-trimethyl-3-[(1-oxohexadecyl)amino]-, chloride (1:1)

## Assessment statement (CA09983)

**13 February 2025**

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# AICIS assessment (CA09983)

## Chemical in this assessment

| Name | CAS registry number |
|---|---|
| 1-Propanaminium, *N*,*N*,*N*-trimethyl-3-[(1-oxohexadecyl)amino]-, chloride (1:1) | 51277-96-4 |

## Reason for the assessment

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

### Certificate application type

AICIS received the application in a Health and Environment Focus type.

## Defined scope of assessment

The chemical has been assessed:

- as imported into Australia at up to 3 tonnes/year
- as imported at approximately 65% concentration for local reformulation of aerosol deodorants containing the assessed chemical at < 1% concentration for use by consumers
- as imported in roll-on deodorant at < 1% concentration for use by consumers

## Summary of assessment

### Summary of introduction, use and end use

The assessed chemical will not be manufactured in Australia. It will be imported as a liquid at approximately 65% concentration in 193 kg drums for local reformulation into aerosol deodorants.

Following the reformulation process, the mixture containing the assessed chemical at < 1% concentration is filled directly into 150 mL, 200 mL and 250 mL aerosol deodorant cans.

The assessed chemical will also be imported in finished roll-on deodorants at < 1% concentration in ready-to-sell 50 mL packs, which will be distributed via road and/or rail to customer warehouses and retail outlets.

Finished roll-on and aerosol deodorants will be widely available to consumers via retail outlets.

# Human health

## Summary of health hazards

The submitted toxicological data on the assessed chemical and on analogue chemicals (see **Supporting information**) indicate that the assessed chemical is:

- of low acute oral and dermal toxicity (LD50 (oral) > 2,000 mg/kg bw in rats, LD50 (dermal) = 4,214 mg/kg bw in rabbits)
- slightly irritating to skin
- considered to cause serious eye damage
- not a skin sensitiser
- not considered to be genotoxic

Analogue data were provided for short-term repeated dose oral and dermal toxicity studies, with doses up to 300 mg/kg bw/day (oral) and up to 10 mg/kg bw/day (dermal) in rats. The effects observed in both studies were due to irritation nature of the analogues. No systemic toxicity effects were observed at up to the highest tested doses in both studies.

No acute or repeated dose inhalation toxicity studies were submitted for the assessed chemical.

## Hazard classifications relevant for worker health and safety

Based on the data provided by the applicant, the assessed chemical satisfies the criteria for classification according to the *Globally Harmonized System of Classification and Labelling of Chemicals* (GHS) (UNECE 2017) for hazard classes relevant for worker health and safety as adopted for industrial chemicals in Australia.

| Health hazards | Hazard category | Hazard statement |
|---|---|---|
| Serious eye damage/eye irritation | Eye Damage 1 | H318: Causes serious eye damage |

## 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 < 1% concentration through the use of aerosol and roll-on deodorants. The principal route of exposure will be dermal, while ocular and inhalation exposures are also possible, particularly from aerosol deodorant.

The assessed chemical is considered to cause serious eye damage (Category 1). However, at the proposed low end use concentrations of the assessed chemical (< 1% concentration) in deodorants, eye damage or irritation hazards to the general public is not expected.

The repeated dose toxicity potential of the assessed chemical was estimated by calculating the margin of exposure (MoE). Using a maximum use concentration of 0.99% in deodorants and a dermal absorption of 100%, a daily systemic exposure to the assessed chemical (including inhalation exposure) of 0.25 mg/kg bw/day was estimated (see **Supporting information** section). Using a no-observable-adverse-effect-level (NOAEL) of 300 mg/kg bw/day, which was derived from a repeated dose oral toxicity study on an analogue chemical

in rats, the MoE was estimated to be 1189. 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.

**Workers**

Potential exposure of workers to the assessed chemical at approximately 65% concentration in liquid form may occur during reformulation processes and quality control (see **Supporting information** section). The principal routes of exposure will be dermal and ocular. Inhalation exposure to the assessed chemical is not expected during reformulation due to the low vapour pressure.

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

## Environment

### Summary of environmental hazard characteristics

According to the *Australian Environmental Criteria for Persistent, Bioaccumulative and/or Toxic Chemicals* (DCCEEW, 2022) and based on the available data the assessed chemical is:

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

### Environmental hazard classification

The assessed 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 2 (H411) based on toxicity data for fish, invertebrates and algae.

| 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 2 | H411: Toxic to aquatic life with long-lasting effects |

### Summary of environmental risk

The assessed chemical will be introduced as a cationic surfactant for use in cosmetic products. This use may result in the release of the assessed chemical to sewers. Consequently, the assessed chemical will be treated at sewage treatment plants (STPs) before release to surface waters.

The assessed chemical is readily degradable and is not persistent, does not have potential for bioaccumulation but is toxic to aquatic organisms.

Although the assessed chemical is toxic according to the *Australian Environmental Criteria for Persistent, Bioaccumulative and/or Toxic Chemicals* (DCCEEW, 2022), it does not meet all three PBT criteria. It is unlikely to cause 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, 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 classifications relevant to work health and safety (see **Hazard classifications relevant for worker health and safety**).

### Information relating to safe introduction and use

The information in this statement, including recommended hazard classifications, should be used by a person conducting a business or undertaking at a workplace (such as an employer) to determine the appropriate controls under the relevant jurisdiction Work Health and Safety laws.

The following control measures could be implemented to manage the risk arising from exposure to the assessed chemical during reformulation:

- Use of engineering controls such as
    - Enclosed and automated systems
    - Adequate workplace ventilation to avoid accumulation of dusts, mists or aerosols
- Use of safe work practices to
    - Avoid contact with skin and eyes
    - Avoid inhalation of dust, mists or aerosols
- Use of personal protective equipment (PPE)
    - Impervious gloves
    - Protective clothing
    - Safety glasses/goggles or face mask
    - 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 2023) or relevant State or Territory Code of Practice.

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

## Conclusions

The Executive Director is satisfied that the risks to human health or the environment associated with the introduction and use of the industrial chemical can be managed.

Note:

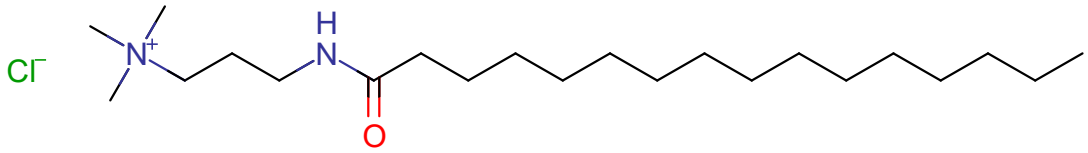
1. Obligations to report additional information about hazards under s 100 of the *Industrial Chemicals Act 2019* apply.
2. You should be aware of your obligations under environmental, workplace health and safety and poisons legislation as adopted by the relevant state or territory.

# Supporting information

## Chemical identity

| | |
|---|---|
| **CAS number** | 51277-96-4 |
| **CAS name** | 1-Propanaminium, *N*,*N*,*N*-trimethyl-3-[(1-oxohexadecyl)amino]-, chloride (1:1) |
| **Molecular formula** | $C_{22}H_{47}N_2O.Cl$ |
| **Molecular weight (g/mol)** | 391.08 |
| **SMILES (canonical)** | [Cl-].O=C(NCCC[N+](C)(C)C)CCCCCCCCCCCCCCC |

**Structural formula**




**Additional chemical identity information**

The assessed chemical has a typical purity between 90 and 95%.

## Relevant physical and chemical properties

| | |
|---|---|
| **Physical form** | White solid |
| **Melting point** | 89-98 °C at 101.3 kPa |
| **Density** | 1,029 kg/m$^3$ at 20 °C |
| **Vapour pressure** | < 0.1 kPa at 20 °C |
| **Water solubility** | 0.203 g/L at 20°C * |
| **Flash Point** | 108 °C ** |
| **Ionisable in the environment** | Yes |
| **log $K_{oc}$** | 4.99 |

* Determined as the critical micelle concentration (CMC), as appropriate for surface active substances

** Product containing the assessed chemical at approximately 60% concentration was tested in study

# Human exposure

## Workers

### Reformulation

During reformulation, the assessed chemical at approximately 65% concentration in liquid form is blended with other raw cosmetic materials using engineering controls and automated process in an enclosed system with adequate ventilation to form the finished cosmetic products. Subsequently, the reformulated products containing the assessed chemical at < 1% concentration is directly transferred to a filling machine for automative filling, which doses the mixture into 150 mL, 200 mL or 250 mL aerosol cans. The aerosol cans are then filled with hydrocarbon propellants and sealed. Samples of products containing the assessed chemical may be taken for quality control purposes during the reformation process. According to the applicant, safe work practices will also be used to avoid any contact with skin or eyes and inhalation through the use of PPE.

Dermal, ocular, and inhalation exposure to the assessed chemical at up to 65% may occur during reformulation activities and quality control. However, as noted above, exposure to the assessed chemical at up to 65% concentration will be minimised through the use of engineering controls and PPE for workers (such as coveralls, impermeable gloves, eye protection, and respiratory protection).

## Public

There will be widespread and repeated exposure of the public to the assessed chemical at < 1% concentration in aerosol and roll-on deodorants. The principal route of exposure will be dermal, while ocular and inhalation exposures are also possible.

Data on typical use patterns of deodorants show an application amount of 1,500 mg/day (SCCS 2012). For the purposes of the exposure assessment, Australian use patterns of deodorants are assumed to be similar to those in Europe. A worst-case dermal absorption (DA) rate of 100% was used along with an average lifetime bodyweight for males and females combined (BW) of 60 kg (enHealth 2012) for calculation purposes. A daily systemic dermal exposure of 0.25 mg/kg bw/day was calculated according to the following formula with a maximum use concentration of 0.99% and a retention factor (RF) of 1:

Daily systemic exposure = (Amount × Concentration × RF × DA)/BW

For the inhalation exposure assessment from the use of aerosol deodorants, 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 for the calculation of the daily systemic inhalation exposure. It was conservatively assumed that the fraction of the assessed chemical inhaled is 50%. The following table provides information on the estimated inhalation exposure obtained using these parameters.

| | | |
|---|---|---|
| Amount of deodorant applied | 1.43 | g/day |
| Maximum intended concentration of the chemical | 0.99 | % |
| Inhalation rate of the user | 20 | $m^3$/day |

| | | |
|---|---|---|
| Exposure duration in zone 1 | 1 | minutes |
| Exposure duration in zone 2 | 20 | minutes |
| Fraction inhaled by the user | 50 | % |
| Volume of zone 1 | 1 | $m^3$ |
| Volume of zone 2 | 10 | $m^3$ |
| Daily systemic exposure | **0.0049** | mg/kg bw/day |

C = maximum intended concentration of assessed chemical
Total daily systemic exposure = Daily systemic exposure in zone 1 [(amount × C × inhalation rate × exposure duration (zone 1) × fraction inhaled)/(volume (zone 1) × body weight)] + Daily systemic exposure in zone 2 [(amount × C × inhalation rate × exposure duration (zone 2) × fraction inhaled)/(volume (zone 2) × body weight)]

The worst-case scenario estimation using these assumptions is for a person who is a simultaneous user of roll-on and aerosol deodorants containing the assessed chemical. This would result in a combined internal dose of 0.25 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 aerosol deodorant) may occur. However, it is considered that the combination of the conservative aerosol deodorant inhalation exposure assessment parameters, and the aggregate exposure from use of dermally roll-on deodorants, which assumes a conservative 100% absorption rate, is sufficiently protective to cover additional inhalation exposure to the assessed chemical from use of other spray cosmetic and household products with lower exposure factors (e.g., air fresheners).

# Health hazard information

The assessed chemical is a surfactant and a quaternary ammonium compound, which is part of the larger trimonium family. The applicant has not provided information on some toxicological endpoints for the assessed chemical in support of this application. In this regard, the applicant has provided a draft amended report of the Cosmetic Ingredient Review (CIR) Expert Panel on the Safety Assessment of Trimoniums (CIR 2010) and the final CIR report on the 'Safety Assessment of Trimoniums as Used in Cosmetics' (Becker et al. 2012).

## Acute toxicity

### Oral

The acute oral LD50 of an analogue chemical was > 2,000 mg/kg bw for acetamidoethyl PG-trimonium and 490 to 5,000 mg/kg bw for straight- and branched-chain alkyl trimoniums. A mixture of cetrimonium and steartrimonium chloride had an acute oral LD50 of > 2,000 mg/kg bw in rats. The acute oral LD50 of laurtrimonium chloride in rats was 490 mg/kg bw in one study and 560 mg/kg bw in the second study. The acute oral LD50 was reported to be between 3,150 and ≥ 5,000 mg/kg bw for choline chloride in rats. For behenoyl PG-trimonium chloride, the acute oral LD50 was reported as 3,700 and > 2,000 mg/kg bw for rats. The acute oral LD50 of acetamidoethyl PG-trimonium for rats was reported to be > 2,000 mg/kg bw.

While there are some outliers in the above results (LD50 around 490-560 mg/kg bw) and no further details were available, based on the above results, the assessed chemical is expected to be of low acute oral toxicity (LD50 > 2,000 mg/kg bw).

### Dermal

In a non-guideline study, an analogue chemical (cetrimonium chloride, undiluted, purity not provided) at 4.3 mL/kg bw (4,214 mg/kg bw) was applied under occlusion to intact or abraded skin of New Zealand White Rabbits (n = 3/sex) for 24 hours and then washed off. All rabbits exhibited normal behaviour until day 3 when the rabbits became lethargic, had depressed reflexes, and were cold to the touch. While they defecated little or none, clear fluid was coming from their noses and mouths. There was reddening of the nictitating membranes and eyelids. There was substantial weight loss; no further information is available in this regard.

Skin irritation was noted after 24 hours of exposure, including slight to severe erythema, moderate or severe oedema, and whitening of the skin. On day 3, there was moderate or severe atonia and moderate or marked coriaceous skin from day 2. Fissuring was observed in three rabbits and desquamation in one rabbit. The study stated that 50% of the rabbits died at the only dose administered. Necropsy revealed brown, liquid faecal matter; lungs adhered to the chest wall and filled with white granular pockets; enlarged gall bladder; and brownish or clear fluid around the nose and mouth. No visible lesions were observed in the rabbits that survived the 14-day observation period. Under the conditions of this study, the acute dermal LD50 value for the analogue chemical, cetrimonium chloride, was 4,214 mg/kg bw. Therefore, the assessed chemical is of low acute dermal toxicity.

## 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) (EpiSkin™ kits) (OECD TG 439). The relative mean viability of the assessed chemical-treated tissues was 98% after the 15 minutes exposure period (followed by 42 hours post-exposure incubation period). This value is well above the ≤ 50% threshold for irritancy. Under the conditions of this study, the assessed chemical is not classified as a skin irritant, according to the GHS criteria.

In another skin irritation study (OECD TG 404), the undiluted assessed chemical was applied under semi-occlusive conditions to the shaved skin of 3 male and 3 female New Zealand albino rabbits for 4 hours. Animals were observed for 72 hours after patch removal. Very slight erythema was observed in one male and one female animal at 24 hours after the application; all effects were resolved at 48 and 72 hours. There was no oedema throughout the study. There were no other signs of irritation. Under the conditions of this study, the assessed chemical was slightly irritating to the skin and not classified as skin irritant, according to GHS criteria.

### Eye irritation

In an eye irritation study, the assessed chemical (30% concentration) was instilled into the conjunctival sac of one eye of 3 male and 6 female albino New Zealand rabbits (OECD TG 405). The treated eyes in 3 animals (washed eyes) were rinsed with room temperature deionized water for one minute beginning 30 seconds after treatment. In the remaining 6 animals, the treated eyes were rinsed with room temperature deionized water for one minute immediately after recording the 24-hour observation. Eye irritation was assessed at 1, 24, 48, 72 hours and at days 4 and 7 following instillation.

In the non-washed eye group, fluorescein staining was observed in all six eyes at 48 hours after treatment and persisted in all six animals through day 7. Corneal opacity and effects on

iris were not possible to score at 1 and 24 hours in all 6 animals due to the severity of chemosis. Corneal opacity, grade 1 (4/6 animals) and 2 (2/6 animals), was observed at 48 hours observation. Corneal opacity (grade 2) was present in 3/6 animals and grade 1 in 3/6 animals from days 3 to 7.

Iris scores were 0 in all six animals at 48 hours observation, grade 1 at the 72 hours observation in 3/6 animals, zero at day 4 in all 6 animals, and was still present (grade 1) in 1/6 animals after 7 days. Conjunctival redness of varying grades (mostly of grade 2 and 3) was present in all six animals at 1 hour and was still present in all 6 animals on day 7.Conjunctival chemosis was observed in 3/3 animals at the 1-hour observation, grade 2 chemosis in 3/3 animals at the 24 hours observation, grade 1-2 chemosis was observed at 48 hours, 72 hours and at day 4, and was still present in 2/3 animals at the end of the observation period on day 7. Grade 1-3 discharge was observed throughout the study period and was still present at the end of the observation in 5/6 animals on day 7.

In addition to the above observations, the maximum mean average irritation score of 45.8 was calculated for day 3 (72 hours) observation and maximum mean scores of 42.3 and 41.5 were also noted for day 4 and 7 observations. According to the study authors, a maximum average score of 45.8 for 30% concentration indicates that the assessed chemical is severely irritating to the eyes.

The authors noted that the reversibility of eye irritation cannot be judged in this case as the study was terminated on day 7. However, as per the eye lesion and the maximum average score on day 7 (41.5), a significant eye irritation was still present at day 7.

Under the conditions of this study, the assessed chemical is classified as Category 1 eye irritant (H318: Causes severe eye damage), according to GHS criteria.

## Sensitisation

The skin sensitisation potential of the assessed chemical was tested using the Buehler test in female albino Dunkin-Hartley guinea pigs (OECD TG 406). Five males and five females were selected for the study and made into two groups (groups I and II). Group 1 animals served as a naive control group. Animals in Group II (test group) were treated with 400 mg of the analogue chemical (97.8%), moistened with 300 µL deionized water, with epicutaneous induction once weekly for three weeks. After a two weeks rest period, all animals (groups I and II), were challenged epicutaneously at virgin test site with an application of 400 mg of the analogue chemical (97.8%), moistened with 300 µL deionized water.

After challenge, no visible changes of the treated skin sites were observed in the control and test group animals at 24 and 48 h after patch removal. Under the conditions of this study, the assessed chemical was reported to be non-sensitising.

## Repeat dose toxicity

### Oral

In a non-guideline repeat dose oral toxicity study, an analogue chemical (cetrimonium chloride, 24% to 26%) was administered to Sprague-Dawley CD rats (n = 10/sex/dose plus additional 5/sex in high dose recovery group) at 0, 30, 100, and 300 mg/kg bw/day in distilled water by gavage 5 days/week for a total of 23 or 24 applications. The recovery group was observed for further 27 days after the treatment.

There was no effect on survival, food consumption, body weight, clinical chemistry and haematological parameters. No treatment related effects observed at ophthalmological examination. There was a slight increase in absolute and relative adrenal weights and a decrease in absolute and relative spleen weights in males; no further information was available on these changes. A thickening of the forestomach mucosa, associated with oedema and sporadic ulceration in males and females in the high-dose group, were noted at necropsy. Microscopic examination revealed inflammatory oedema in the forestomach mucosa, sporadic ulceration, and acanthosis up to papillomatous hyperplasia in both sexes in the high-dose group. No histopathological or microscopic alterations were observed in the 30 and 100 mg/kg bw/day groups. All treatment-related effects were reversed following the recovery period.

As noted by the authors, the effects observed in this study could be due to the irritation nature of the analogue chemical. However, the forestomach issues reported in this study are considered as not relevant to humans as human do not have a forestomach. As no adverse systemic toxicity effects were reported up to the maximum tested dose, the NOAEL for the analogue chemical was considered to be 300 mg/kg bw/day. Therefore, the assessed chemical is considered to have a similar or higher NOAEL for systemic toxicity.

### Dermal

In a non-guideline repeated dose dermal toxicity study, an analogue chemical (cetrimonium chloride, 54% in aqueous isopropanol) was dermally applied to the clipped skin of New Zealand White rabbits (n = 5/sex/dose) for 5 days/week for 4 weeks at 0% and 0.5%, and at 0 mg/kg bw/day and 10 mg/kg bw/day. Skin was abraded with a clipper head prior to each application. Treated skin was cleaned with water after 6.5 to 7 hours (no further information is available for this aspect). Two control rabbits died during the study.

No treatment related effects were noted on body weight, haematology, organ weight, gross necropsy findings, or histopathology. However, mild to marked acanthosis with active mitosis, hyperkeratosis, and necrosis of the epidermis and hair follicles, with some encrustation and exudates were noted on treated areas of skin.

Slight to moderate erythema was observed in all treated rabbits from days 4 to 8, disappeared in 4 rabbits by day 17. Very slight to slight oedema was observed from days 6 to 12 in 4 rabbits, subsided by day 17. There was intermittent slight oedema during week 4 in 2 rabbits; and 1 rabbit developed oedema on day 20. Three rabbits had slight atonia up to week 4. Slight skin fissuring was observed in most of the treated rabbits that typically disappeared by the end of the study.

The authors noted that the Scientific Committee on Cosmetic Products (SCCP) concluded that the skin effects in this study were due to local irritation and there was not any evidence of systemic toxicity. Under the conditions of this study and based on the lack of systemic toxicity at the highest treated dose, the authors concluded that the dermal no observed effects level (NOEL) was 10 mg/kg bw/day for the analogue chemical.

## Genotoxicity

The assessed chemical was not mutagenic in a bacterial reverse mutation assay using *Salmonella typhimurium strains*, TA97a, TA98, TA100, and TA1535, with or without metabolic activation (OECD TG 471). There was no evidence of increase in the number of revertant colonies that exceeded twice the background level in any of the five tester strains investigated at dose levels up to 0.01 mg/plate in the absence of S9 or at dose levels up to 0.05 mg/plate

in the presence of S9. There was no evidence of induced mutant colonies over background levels. Under the conditions of the study, the assessed chemical was not mutagenic.

In a non-guideline study, an analogue chemical (laurtrimonium chloride) (0.0038 - 0.050 µl/mL without metabolic, 0.012 - 0.16 µL/mL with metabolic activation) was tested negative for its potential to induce mutations at the mouse lymphoma thymidine kinase (TK) locus in mouse lymphoma L5178Y cells (Becker et al. 2012).

In an in vitro chromosome aberration study (non-guideline), an analogue chemical (cetrimonium chloride) was incubated with V79 Chinese hamster cells at 24% - 26%, using concentrations of 0.1 - 6.0 µL/mL without metabolic activation; 0.1 - 10.0 µL/mL with metabolic activation. There were no increases in the number of cells with structural aberrations at any concentration with or without metabolic activation (Becker et al. 2012).

# Environmental exposure

The assessed chemical is a cationic surfactant used as a cosmetic ingredient to be included in deodorants only. Use of these deodorants will 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.

A large part of the assessed chemical will be imported within formulated personal care products, and a smaller portion will be brought into Australia for reformulation into cosmetic products. Reformulation involves weighing the chemical and adding it to the mixing tank, followed by automated filling of the reformulation products into containers. The blending and filling processes occur in enclosed systems.

There will be no direct discharge to the environment during reformulation. Residues in plastic storage drums are sealed and disposed of in landfill. Residues from the blending process are washed out and are discharged into the on-site STP.

Positively charged compounds are expected to react with negatively charged waste to form solids, which precipitate, are collected as sludge and disposed of in landfill. In case of an accidental spill, the chemical will be collected for disposal in accordance with relevant Local, State, Territory and Federal regulations.

## Environmental fate

### Dissolution, speciation and partitioning

The assessed chemical in this assessment is expected to partition to water and sediment when released into the environment.

The assessed chemical is a quaternary ammonium salt, and as an ionic organic chemical it is expected to dissociate in environmental waters (pH 4-9) and release its cation. The chemical is moderately soluble in water (water solubility/CMC = 0.203 g/L at 20°C) and is surface active. Thus, it is expected to partition to the phase boundary when released to the environment.

Carbon soil adsorption coefficients ($K_{OC}$) of 45,361–183,082 L/kg indicate that the chemical will be immobile and will preferentially adsorb to phases in the environment with high organic carbon content (including sediment and soil).

### Degradation

The assessed chemical is expected to be readily degradable in the environment.

A ready biodegradation experiment conducted according to OECD test guideline (TG) 301B found that the substance is degradable to 100% (CO2 evolution) under screening test timeframes of 28 days, fulfilling the 10-day window criterion.

An aerobic sewage treatment simulation test according to OECD TG 303A found that elimination of the test item from effluent in a continuously operating activated sludge unit was 99.29%, and that the main elimination process is biodegradation.

The assessed chemical contains a hydrolysable functionality (amide), which is not expected to rapidly hydrolyse under environmental conditions.

### Bioaccumulation

The assessed chemical is expected to exhibit a low potential to accumulate in aquatic organisms. Read-across measured bioconcentration factors (BCFs) for similar chemicals are below the domestic categorisation threshold for bioaccumulation.

The assessed chemical is not expected to bioaccumulate due to its surfactant properties and ready biodegradability. Surfactants tend to be retained on epithelial surfaces rather than cross cellular membranes. BCFs have been read across from similar quaternary ammonium surfactants, for which measured BCFs ranged between 13–741 L/kg and are below the domestic categorisation thresholds for bioaccumulation.

## 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 large proportion (87%) of the assessed chemical will undergo biodegradation and limited adsorption to sludge is expected. Total removal during STP treatment is estimated to be 87%. Therefore, 13% 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 | 3,000 | kg/year |
| Proportion expected to be released to sewer | 100% | |
| Annual quantity of chemical released to sewer | 3,000 | kg/year |
| Days per year where release occurs | 365 | days/year |
| Daily chemical release | 8.22 | kg/day |

| | | |
|---|---|---|
| Water use | 200.0 | L/person/day |
| Population of Australia | 25.423 | million |
| Removal within STP | 87% | mitigation |
| Daily effluent production | 5,085 | ML/day |
| Dilution Factor - River | 1.0 | |
| Dilution Factor - Ocean | 10.0 | |
| PEC - River | 0.21 | µg/L |
| PEC - Ocean | 0.02 | µg/L |

# Environmental effects

## Effects on aquatic Life

### Acute toxicity

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

| Taxon | Endpoint | Method |
|---|---|---|
| **Fish** | 96 h LC50 = 0.0455 mg/L | *Danio rerio* (zebrafish)<br>OECD TG 236<br>Semi-static conditions<br>in river water<br>Measured concentration |
| **Invertebrate** | 48 h EC50 = 0.0614 mg/L | *Daphnia magna* (water flea)<br>Immobilisation<br>OECD TG 202<br>Semi-static conditions<br>in river water<br>Measured concentration |
| **Algae** | 72 h EC50 = 0.424 mg/L | *Desmodesmus suspicatus* (green algae)<br>Growth<br>OECD TG 201<br>Static conditions<br>in river water<br>Measured concentration |

### Chronic toxicity

The following measured no-observed effect concentration (NOEC) value for one model organism was supplied for the assessed chemical:

| Taxon | Endpoint | Method |
|---|---|---|
| **Algae** | 72 h NOEC = 0.021 mg/L | *Desmodesmus suspicatus* (green algae)<br>Growth<br>OECD TG 201<br>Static conditions<br>in river water<br>Measured concentration |

## Predicted no-effect concentration (PNEC)

A predicted no-effect concentration (PNEC) of 0.455 µg/L was calculated for the assessed chemical in the aquatic environment. This value was derived using the endpoint value for algae (0.00455 mg/L). An assessment factor of 100 was applied to this endpoint as acute toxicity data were provided for all three trophic levels and chronic toxicity data were 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 the *Australian Environmental Criteria for Persistent, Bioaccumulative and/or Toxic Chemicals* (DCCEEW, 2022) is presented below:

## Persistence

Not Persistent (Not P). Based on measured degradation studies, the assessed chemical is categorised as Not Persistent.

## Bioaccumulation

Not Bioaccumulative (Not B). Based on low measured read-across bioconcentration factors (BCF) in fish, the assessed chemical is categorised as Not Bioaccumulative.

## Toxicity

Toxic (T). Based on available ecotoxicity values below 1 mg/L and evidence of high chronic toxicity, 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 | 0.21 µg/L | 0.455 | 0.462 |
| Ocean | 0.02 µg/L | 0.455 | 0.046 |

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

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