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NATIONAL INDUSTRIAL CHEMICALS NOTIFICATION AND ASSESSMENT SCHEME (NICNAS)

FULL PUBLIC REPORT

Isooctadecanoic acid, 1-methylheptyl ester (INCI Name: Methylheptyl isostearate)

This Assessment has been compiled in accordance with the provisions of the *Industrial Chemicals (Notification and Assessment) Act 1989* (Cwlth) (the Act) and Regulations. This legislation is an Act of the Commonwealth of Australia. The National Industrial Chemicals Notification and Assessment Scheme (NICNAS) is administered by the Department of Health and Ageing, and conducts the risk assessment for public health and occupational health and safety. The assessment of environmental risk is conducted by the Department of Sustainability, Environment, Water, Population and Communities.

For the purposes of subsection 78(1) of the Act, this Full Public Report may be inspected at our NICNAS office by appointment only at Level 7, 260 Elizabeth St, SURRY HILLS NSW 2010.

This Full Public Report is also available for viewing and downloading from the NICNAS website or available on request, free of charge, by contacting NICNAS. For requests and enquiries please contact the NICNAS Administration Coordinator at:

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Director
NICNAS

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1. APPLICANT AND NOTIFICATION DETAILS

APPLICANT(S)
Avon Products Pty Ltd (ABN 48 008 428 457)
120 Old Pittwater Road
Brookvale NSW 2100

NOTIFICATION CATEGORY
Limited-small volume: Chemical other than polymer (1 tonne or less per year).

EXEMPT INFORMATION (SECTION 75 OF THE ACT)
No details are claimed exempt from publication.

VARIATION OF DATA REQUIREMENTS (SECTION 24 OF THE ACT)
Variation to the schedule of data requirements is claimed for all the data required under the schedule of data requirements.

PREVIOUS NOTIFICATION IN AUSTRALIA BY APPLICANT(S)
None

NOTIFICATION IN OTHER COUNTRIES
The notifier has stated that the notified chemical has been in use in many countries for a number of years However, the names of countries have not been stated.

2. IDENTITY OF CHEMICAL

MARKETING NAME(S)
Beantree (containing the notified chemical at >97% concentration)
Avon Dream Life Body Lotion (finished product containing the notified chemical at up to 5%)

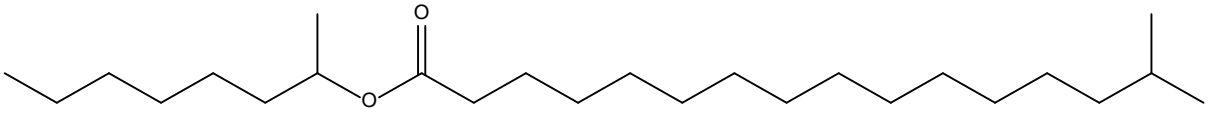
CAS NUMBER
209802-43-7

CHEMICAL NAME
Isooctadecanoic acid, 1-methylheptyl ester

OTHER NAMES
Methylheptyl isostearate, octyl isostearate
Capryl isostearate

MOLECULAR FORMULA
$C_{26}H_{52}O_2$

STRUCTURAL FORMULA



MOLECULAR WEIGHT
Mn = 396.70 Da.

ANALYTICAL DATA

ANALYTICAL METHOD	Infrared (IR) Spectroscopy Major peaks at 2927, 2856, 1736, 1466, 1459, 1420, 1377, 1340, 1301, 1249, 1178, 1120, 1081, 1038 and 723 cm^{-1}
Remarks	The IR Spectra was done on a sample neat between NaCl plates.
TEST FACILITY	Avon Products (1999). PI 10318 Infrared Spectra. Avon Method APAM 8.000-3. Avon Products Inc, 1345 Avenue of the Americas, New York NY 10020. 15 November 1999.

3. COMPOSITION

DEGREE OF PURITY >97%

HAZARDOUS IMPURITIES/RESIDUAL MONOMERS None

NON HAZARDOUS IMPURITIES/RESIDUAL MONOMERS (>1% by weight)

Chemical Name	Heptadecanoic acid, 16-methyl-		
CAS No.	2724-58-5	*Weight %*	≤2%

Chemical Name	2-Octanol		
CAS No.	123-96-6	*Weight %*	≤1%

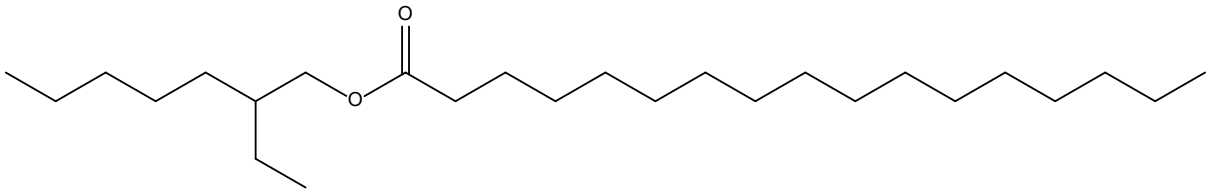
ADDITIVES/ADJUVANTS
None

LOSS OF MONOMERS, OTHER REACTANTS, ADDITIVES, IMPURITIES
None

DEGRADATION PRODUCTS
None

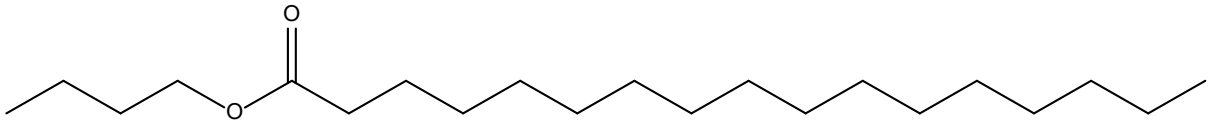
Identity of Analogue Chemicals Used in Estimating the Physical, Chemical, Toxicological and Ecotoxicological Properties of the Notified polymer

Analogue 1 - Octadecanoic acid, 2-ethylhexyl ester (CAS No. 22047-49-0) (Octyl stearate)
Molecular formula = $C_{26}H_{52}O_2$
MW = 396.7 Da.
Structural formula



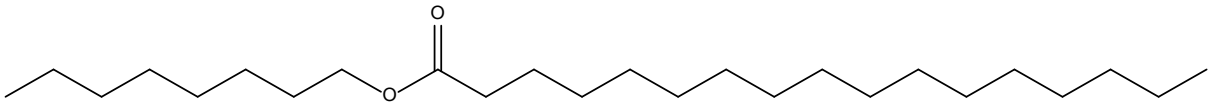
Analogue 1 has an identical molecular weight to the notified chemical, a similar length acid moiety which is a straight chain whereas the notified chemical has an iso-group and an ethyl-branched alcohol moiety whereas the notified chemical has a methyl-branched alcohol moiety (each 8 carbons in length). The differences in the composition of the alkyl components of the analogue chemical when compared to the notified chemical are not significant and therefore, Analogue 1 is expected to be the most suitable analogue for estimating the physical and chemical properties of the notified chemical. Given it has the same molecular weight and reactive functional group as the notified chemical and is expected to have very similar physical and chemical properties, it is also expected to provide a suitable estimation of the likely toxicological properties of the notified chemical.

Analogue 2 - Octadecanoic acid, butyl ester (CAS No. 123-95-5) (Butyl stearate)
Molecular formula = $C_{22}H_{44}O_2$
MW = 340.57 Da.



Analogue 2 has a slightly lower molecular weight than the notified chemical, a similar length acid moiety which is a straight chain whereas the notified chemical has an iso-group and a straight chain alkyl alcohol moiety 4 carbons in length compared to the ethyl-branched alkyl alcohol moiety 8 carbons in length in the notified chemical. Analogue 2 has a slightly lower molecular weight than the notified chemical and therefore it is expected that there will be slight differences between the physical and chemical properties of this analogue and the notified chemical. However, the differences are not expected to be substantial. Analogue 2 is also expected to provide a suitable estimate for toxicological properties of the notified chemical.

Analogue 3 Octadecanoic acid, octyl ester (CAS No. 109-36-4) (2-Ethylhexy stearate)
Molecular formula = $C_{26}H_{52}O_2$
MW = 396.7 Da.



Analogue 3 has an identical molecular weight to the notified chemical with the only structural differences being the straight chain alkyl alcohol moiety 8 carbons in length compared to the ethyl-branched alkyl alcohol moiety 8 carbons in length in the notified chemical; and the straight chain acid moiety 18 carbons in length compared to the acid moiety with an iso-group in the notified chemical. Given the identical molecular weight and similar functionality, Analogue 3 is expected to provide a reasonable estimate of physical and chemical properties as well as toxicological properties. However, it should be noted that there is only limited data available on Analogue 3.

4. PHYSICAL AND CHEMICAL PROPERTIES

APPEARANCE AT 20°C AND 101.3 kPa: Amber liquid with a fatty odour

The data below were either taken from the MSDS for the notified chemical, analogue 1 or 2 or based on estimates.

Property	Value	Data Source/Justification
Melting Point	20°C	Analogue 1
Boiling Point	416°C	Estimated (EPIsuite v4.0, 2009)
Density*	855-865 kg/m^3 at 25°C	MSDS
Vapour Pressure	4.42 x 10^{-5} Pa at 25°C	Estimated using MPBVP (v1.43)
Water Solubility	4.65 x 10^{-10} to 7.55 x 10^{-10} g/L at 25°C	Estimated using WSKOW (v1.41)
Hydrolysis as a Function of pH	Not determined	The notified chemical contains hydrolysable functionality, however, based on its estimated low water solubility, hydrolysis is expected to be very slow in the environmental pH range (4-9) at ambient temperature
Partition Coefficient (n-octanol/water)	log K_{ow} = 11.52	Estimated using KOWWIN (v1.67)
Adsorption/Desorption	log K_{oc} = 6.37 to 7.23	Estimated using KOCWIN (v2.00)
Dissociation Constant	Not determined	The notified chemical does not contain functional groups that are expected to dissociate under typical environmental conditions

Particle Size	Not measured	The notified chemical is a liquid.
Flash Point*	212°C	MSDS
Flammability	Not expected to be flammable	Estimated based on chemical structure
Autoignition Temperature	355°C	Analogue 2
Explosive Properties	Not predicted to be explosive	Estimated based on chemical structure

* Data sourced from MSDS for Beantree (containing the notified chemical at >97% concentration)

DISCUSSION OF PROPERTIES

Reactivity
The notified chemical is chemically stable and will not decompose under normal ambient conditions.

Dangerous Goods classification
Based on the submitted physical-chemical data in the above table the notified chemical is not classified according to the Australian Dangerous Goods Code (NTC, 2007). However the data above do not address all Dangerous Goods endpoints. Therefore consideration of all endpoints should be undertaken before a final decision on the Dangerous Goods classification is made by the introducer of the chemical.

5. INTRODUCTION AND USE INFORMATION

MODE OF INTRODUCTION OF NOTIFIED CHEMICAL (100%) OVER NEXT 5 YEARS
The notified chemical will be imported in finished cosmetic, skin and hair care products at up to 5% concentration.

MAXIMUM INTRODUCTION VOLUME OF NOTIFIED CHEMICAL (100%) OVER NEXT 5 YEARS

Year	*1*	*2*	*3*	*4*	*5*
Tonnes	1	1	1	1	1

PORT OF ENTRY
Sydney

IDENTITY OF RECIPIENTS
Avon Products Pty Ltd

TRANSPORTATION AND PACKAGING
The notified chemical will be imported at up to 5% concentration in cosmetic, skin and hair care products in 200 mL bottles and tubes suitable for retail sale. The product containers will be packaged in cartons and 12 cardboard cartons will be packed in a cardboard shipper. Products will be transported from the wharf to the notifier's warehouse for storage and subsequent distribution.

USE
The notified chemical will be used as an emollient in finished cosmetic, skin and hair care products at up to 5% concentration. Examples of products which may contain the notified chemical include: shampoos, conditioners, cleansing products foams, fragrances, skin creams and lotions for facial and body care, bath and shower products, sunscreens, antiperspirants and deodorants.

OPERATION DESCRIPTION
The notified chemical will be imported in finished cosmetic, skin and hair care products at up to 5% concentration. The finished products containing the notified chemical at up to 5% will be transported from the wharf to the distribution centre and stored in the warehouse. From these depots, the products will be transported to retail outlets for sale to consumers as well as health and beauty salons. Workers in hair and beauty salons will directly apply finished products containing the notified chemical at up to 5% concentration to clients.

6. HUMAN HEALTH IMPLICATIONS

6.1 Exposure assessment

6.1.1 Occupational exposure

NUMBER AND CATEGORY OF WORKERS

Category of Worker	*Number*	*Exposure Duration (hours/day)*	*Exposure Frequency (days/year)*
Transport and storage	10	4	12
Store persons	2	4	12
End users	$3x10^5$	8	365

EXPOSURE DETAILS

Transport and Storage

Exposure to the notified chemical during transport and storage is not anticipated except in case of an accident leading to release.

Use of finished personal care products

Occupational exposure is possible for workers in hair and beauty salons using products containing the notified chemical (up to 5%). Dermal exposure is expected to be extensive given that cosmetic, skin and hair care products containing the notified chemical will be applied directly to the skin and hair. Accidental ocular exposure and oral ingestion may also occur.

Although the level and route of exposure will vary depending on the method of application and work practices employed, extensive dermal exposure is expected in some occupational settings. This exposure is likely to be greater than that expected for the public (see below).

6.1.2. Public exposure

Public exposure to the notified chemical is expected to be widespread and frequent through daily use of cosmetic, skin and hair care products containing the notified chemical at concentrations up to 5%. Exposure to the notified chemical will vary depending on individual use patterns. The principal route of exposure will be dermal, while ocular and inhalation exposure is also possible, particularly if products are applied by spray. Accidental ingestion from the use of these types of products is also possible from facial use.

Public exposure to the notified chemical in Australia has been estimated using the Scientific Committee on Consumer Products' (SCCP's) Notes of Guidance for the Testing of Cosmetic Ingredients and their Safety Evaluation (SCCP, 2006) and applying the following assumptions:

- Bodyweight of 60 kg for females (SCCP, 2006);
- Concentration of the notified chemical in rinse off cosmetic products: 5%;
- Concentration of the notified chemical in leave on cosmetic products: 5%;
- 100% dermal absorption (SCCP, 2006);
- An individual uses all product types containing the notified chemical.

Product(s) used	*Use level for each product (g)*	*Retention factor*	*Systemic Exposure (mg/kg bw/day)*
Rinse-off			
Facial cleanser[1]	2.5 x 2 applications/day	0.01	0.83
Shampoo	8.0 x 1 application/day	0.01	1.33
Conditioner	14.0 x 0.28 applications/day	0.01	0.65
Shower gel	5.0 x 2 applications/day	0.01	1.67
Makeup remover	2.5 x 2 applications/day	0.10	8.33
Total rinse-off product exposure =			12.82
Leave-on			
Body Lotion	8.0 x 1 application/day	1.0	133.33
Face Cream	0.8 x 2 applications/day	1.0	26.67
General purpose cream			

Total leave-on product exposure =	160.00
Total Systemic Exposure (rinse-off + leave-on x conc. in each product) = (172.82 mg/kg bw/day x 5%)	**8.64**

[1]RIVM (2006)

The above exposure estimate was produced using highly conservative assumptions and is expected to reflect a worst-case scenario. However, in reality, the level of exposure is expected to be lower than 8.64 mg/kg bw/day as it is assumed that consumers would not use all these products to the extent shown above, and dermal absorption may be less than 100%.

6.2. Human health effects assessment

No toxicity data were submitted on the notified chemical itself. However, toxicological data on 3 analogues is presented below.

Endpoint	*Analogue 1*	*Analogue 2*	*Analogue 3*
Rat, acute oral toxicity (LD50)	>8 mL/kg bw	>32 g/kg bw	>8 mL/kg bw
Rabbit, skin irritation	Slightly irritating	irritating	Not available
Rabbit, eye irritation	Slightly irritating	Non irritating	Not available
Rabbit, skin irritation (repeated application)	Signs of irritation at 100% and 10%	Not available	Not available
Guinea pig, skin sensitisation – adjuvant test	Not available	No evidence of sensitisation	Not available
Human, repeat insult patch test	Non irritating at 7.6%	Non irritating at 50% and 10%	Not available
Human, skin sensitisation	Non sensitising at 7.6%	Non sensitising at 50% and 10%	Not available
Phototoxicity	Non phototoxic	Not available	Not available
Photosensitisation	Not a photosensitiser	Not a photosensitiser	Not available
Rat, repeat dose oral toxicity – 28 days (mg/kg bw/day)	Not available	Not available	NOAEL = 1000
Rat, chronic oral toxicity – 2 years (mg/kg bw/day)	Not available	NOAEL = 6250	Not available
Mutagenicity – bacterial reverse mutation	Not available	Non mutagenic	Non mutagenic
Developmental and reproductive effects	Not available	NOAEL = 6.25%	NOAEL = 1000 mg/kg bw/day

Toxicokinetics and metabolism

The notified chemical is expected to readily undergo hydrolysis to form the corresponding alcohol (1-Methylheptanol) and carboxylic acid (Octadecanoic acid or Stearic acid). These are expected to either be stored in tissues in the form of triglycerides or undergo oxidization to form carbon dioxide and water (CIR, 1985).

Acute toxicity

The notified chemical is expected to be of low acute oral toxicity based on the low acute oral toxicity of analogues (CIR, 1985).

Neither the notified chemical nor its analogues were tested for acute dermal or acute inhalation toxicity. However, the estimated low water solubility and high log Pow (based on analogue data) are expected to limit dermal penetration. The estimated low vapour pressure is expected to limit the potential for inhalation.

Irritation and Sensitisation

The highest primary irritation index (PII) score for Analogue 2 was reported to be 2.75 which was observed following occluded application to intact and abraded skin for 24 hours (CIR, 1985). The following observations were reported on the intact skin: at 24 hours, well-defined to moderate erythema in all animals and very slight edema in 2/6 animals; and at 72 hours: well-defined to severe edema in all animals. The reported skin reactions may be sufficient for classification with R36: irritating to the skin. However, without knowing the score of the reactions at 48 hours, this is uncertain. In other skin irritation studies on Analogue 1 and 2 in rabbits under similar conditions, no or slight irritation was reported. Therefore, as a worst-case estimate, the notified chemical should be considered to have the potential to illicit skin irritation in humans.

Eye irritation tests on Analogues 1 and 2 in rabbits found signs of irritation 1 hour following application (in Analogue 1) but no signs of irritation were observed following this observation point in any of the tests (CIR, 1985). Therefore, the notified chemical should be considered not to be irritating to the eye based on the absence of irritation observed in tests on analogue chemicals.

Analogue 1 was applied undiluted and at 10% concentration to the shaved skin of 3 rabbits each day for 6 days. At the end of the test period, the mean maximum irritation index (MMII) for rabbits treated with Analogue 1 undiluted was 0.67 indicating it was "poorly tolerated". Microscopic examination revealed epidermal acanthosis and congestive dermatitis. The MMI for rabbits treated with Analogue 1 at 10% in aqueous solution was 0.33, indicating it was "relatively well tolerated". Vesicles were observed in 2 of the 3 rabbits but no significant changes were observed during microscopic examination (CIR, 1985). Based on these results in Analogue 1, the notified chemical is considered to have the potential to be irritating following repeated exposure.

Neither the notified chemical nor the analogue chemicals contain a structural alert for skin sensitisation (Barratt et al., 1994).

A skin sensitisation study on Analogue 2 found it not to be sensitising to guinea pigs following intracutaneous injection at a concentration of 0.1% (CIR, 1985). No evidence of skin sensitisation was reported in the test but skin sensitisation at higher concentrations could not be ruled out entirely.

A number of skin irritation, skin sensitisation, phototoxicity and photosensitisation studies have been conducted in human volunteers on Analogues 1 and 2.

A suntan lotion and a protective face cream each containing Analogue 1 at 7.6% concentration was found not to be an irritant or a sensitiser in 56 human volunteers treated with 10 applications (CIR, 1985). The same products containing Analogue 1 at 7.6% were also found not to be phototoxic in 10 volunteers (CIR, 1985). The photosensitisation potential of the two products was also tested in 27 volunteers (CIR, 1985). Reactions were observed in 4 subjects. However, 3 of these were isolated incidents of minor severity that did not persist or reoccur during the challenge phase (CIR, 1985). The fourth subject displayed signs of erythema during the induction phase but this resolved following irradiation. The same reaction was observed at 2 sites during the challenge phase. However, the study authors noted that the reactions were slight and did not attribute significance to them. Therefore, Analogue 1 was also considered to be not photosensitising.

Analogue 2 at a concentration of 50% in mineral oil was found to elicit signs of skin sensitisation in 2/111 volunteers who had the chemical applied to intact skin on the back for 48 hours under a semi-occluded patch followed by a 2-week nontreatment period and a further application for 48 hours under a semi-occluded patch (CIR, 1985). However, the signs did not persist and were considered to be sporadic by the authors of the study (CIR, 1985).

Analogue 2 at 10% concentration in a cosmetic product was also found to be nonirritating, nonsensitising and nonphotosensitising in a repeat insult patch test (RIPT) in 54 female volunteers (CIR, 1985).

Overall, based on the weight of evidence, the notified chemical is not considered to be a skin sensitiser, given the absence of a structural alert for skin sensitisation (Barratt et al., 1994), the findings of a sensitisation study on an analogue in guinea pigs (CIR, 1985) and the lack of significant adverse effects in a range of clinical studies in human volunteers using analogue chemicals (CIR, 1985).

Repeated Dose Toxicity

A chronic oral toxicity study was conducted using Analogue 2 in rats at concentrations of 0%, 1.25% and 6.25% in the diet (equivalent to approximately 0, 1250 and 6250 mg/kg bw/day) (CIR, 1985). Gross lesions, pathological changes and histopathological abnormalities were observed in both treated groups but in the absence of a dose response relationship, they were not considered treatment related. Therefore, the NOAEL for Analogue 2 was considered to be 6500 mg/kg bw/day.

A 28-day repeated dose oral toxicity study in rats using Analogue 3 found it to have a NOAEL of 1000 mg/kg bw/day (US EPA, 2003).

A chronic oral toxicity study on Analogue 2 and a 28-day repeated dose oral toxicity study on Analogue 3 indicate that they are of low subchronic and chronic oral toxicity. Therefore, assuming the slight differences in chemical structure between these analogues and the notified chemical do not result in different metabolic pathways, the notified chemical is also expected to be of low subchronic and chronic oral toxicity.

Mutagenicity
The European Food Safety Authority (EFSA) reported that Analogue 2 was not mutagenic in an Ames test either in the presence or absence of metabolic activation (EFSA, 2007). EFSA also noted that "…uniformly negative results in bacterial and cytogenetic assays are reported in the literature for other fatty acid esters." (EFSA, 2007). A report prepared for the US EPA also reported that Analogue 3 was negative in an Amest test (US EPA, 2003). Based on these reports for similar chemicals, the notified chemical is not considered to be mutagenic or genotoxic.

Reproductive and developmental toxicity
A reproductive study on Analogue 2 at concentrations up to 6.25% in rats fed with the chemical for 10 weeks prior to mating found no adverse effects on fertility, litter size and survival of offspring (US EPA, 2003).

In another study on Analogue 3, the NOAEL for embryo-/fetotoxicity, teratogenicity and maternal toxicity in rats was found to be 1000 mg/kg bw/day (US EPA, 2003).

Based on these result in analogue chemicals, the notified chemical is not considered to be toxic for reproduction or development up to 6.25% concentration or up to 1000 mg/kg bw/day.

Health hazard classification
Based on the available data on analogue chemicals, the notified chemical is not classified as hazardous according to the *Approved Criteria for Classifying Hazardous Substances* (NOHSC, 2004).

6.3. Human health risk characterisation

6.3.1. Occupational health and safety
Employees in hair and beauty salons will experience extensive dermal exposure during application of products containing the notified chemical (<5%) by hand or spray. If these employees use products containing the notified chemical for personal use as well as in a work setting their level of exposure would be higher than that of consumers. Reports on analogue chemicals indicate that there is potential for skin and eye irritation when used undiluted. However, exposure to the notified chemical at low concentrations (<5%) in cosmetic products is not expected to result in irritation. The risk of toxicity following repeated exposure is not anticipated to be unacceptable based on the NOAELs reported in repeat dose oral toxicity studies on analogous chemicals.

6.3.2. Public health
Members of the public will experience widespread and frequent exposure to the notified chemical through daily use of cosmetic products (<5%) which will be applied directly to the skin and hair. At this concentration, the notified chemical is not expected to cause skin or eye irritation.

A maximum systemic exposure of 8.64 mg/kg bw/day was estimated (see Section 6.1.2) for a person using various products containing the notified chemical at 5% concentration at the same time. A NOAEL could not be established for the notified chemical itself, but it can be estimated to be similar to that for Analogue 2 (6500 mg/kg bw/day). Therefore a conservative estimate of the margin of exposure (MoE) for the notified chemical could be estimated as follows:

$$\text{MoE} = \frac{\text{Estimated NOAEL}}{\text{Estimated typical daily systemic exposure}} = \frac{6{,}500 \text{ mg/kg bw/day}}{8.64 \text{ mg/kg bw/day}}$$

$$= 752$$

This MoE > 100 indicates the level of risk for the general public using many products containing the notified chemical at the same time is acceptable.

Overall, based on the available data, the notified chemical is not considered to pose an unreasonable risk to public health at concentrations up to 5% in cosmetic products.

7. ENVIRONMENTAL IMPLICATIONS

7.1. Environmental Exposure & Fate Assessment

7.1.1 Environmental Exposure

RELEASE OF CHEMICAL AT SITE
The notified chemical will be imported as a component of finished cosmetic products. Accidental spills during transport are expected to be collected with inert material and sent to landfill.

RELEASE OF CHEMICAL FROM USE
The notified chemical is a component in rinse-off and leave-on cosmetic products. Therefore, it is expected that the majority of the imported quantity of notified chemical will be released to sewer.

RELEASE OF CHEMICAL FROM DISPOSAL
Residue of the notified chemical in the empty containers (1%) is likely either to share the fate of the container and be disposed of to landfill, or to be washed to sewer when containers are rinsed before recycling.

7.1.2 Environmental fate

No environmental fate data were submitted. However, the notified chemical is predicted to be readily biodegradable by modules of the estimation program BIOWIN (v4.10) (US EPA, 2009). The majority of notified chemical will be disposed of to sewer, where it is likely to partition to the sludge due to its estimated high log K_{oc} (6.37–7.23). Sludge containing the notified chemical may be disposed of to landfill or used for soil remediation. Notified chemical in sludge, soil or landfill is expected to be immobile and to degrade through biotic and abiotic processes to form water and oxides of carbon. Although the notified chemical has a moderate molecular weight and a high calculated log K_{ow} (11.52), calculations with BCFBAF (v3.00) (US EPA, 2009) indicate a low bioconcentration potential (BCF = 20.5 L/kg wet-wt).

7.1.3 Predicted Environmental Concentration (PEC)

Assuming that most of the notified chemical will be washed into the sewer, the following Predicted Environmental Concentration (PEC) in sewage effluent on a nationwide basis was calculated.

Predicted Environmental Concentration (PEC) for the Aquatic Compartment		
Total Annual Import/Manufactured Volume	1,000	kg/year
Proportion expected to be released to sewer	100%	
Annual quantity of chemical released to sewer	1,000	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 (Millions)	21.161	million
Removal within STP	0%	
Daily effluent production:	4,232	ML
Dilution Factor - River	1.0	
Dilution Factor - Ocean	10.0	
PEC - River:	0.65	µg/L
PEC - Ocean:	0.06	µg/L

The notified chemical is predicted to partition to sludge and to be readily biodegradable, hence the removal of >97% of the notified chemical from influent by sewage treatment plant (STP) processes is expected (Simple Treat; European Commission, 2003). However, in this worst case model, the majority of the notified chemical is assumed to be released in effluent. STP effluent re-use for irrigation occurs throughout Australia. The agricultural irrigation application rate is assumed to be 1000 L/m^2/year (10 ML/ha/year). The notified chemical in this volume is assumed to infiltrate and accumulate in the top 10 cm of soil (density 1500 kg/m^3). Using these assumptions, irrigation with a concentration of 0.647 µg/L may potentially result in a soil concentration of approximately 4.316 µg/kg.

Assuming accumulation of the notified chemical in soil for 5 and 10 years under repeated irrigation, the concentration of notified chemical in the applied soil in 5 and 10 years may be approximately 21.58 µg/kg and 43.16 µg/kg, respectively. However, due to the absorptive characteristics of the notified chemical, and its likely biodegradability, these calculated values represent maximum concentrations only.

7.2. Environmental effects assessment

No experimental data were submitted. The notified chemical is not expected to be bioavailable based on its very high predicted log K_{ow} of 11.52. Therefore, no effects on aquatic biota are predicted for the notified chemical at its water saturation concentration (ECOSAR (v1.00), US EPA, 2009). Classification should only be based on toxic responses observed in the soluble range and, therefore, the notified chemical cannot be formally classified under the Globally Harmonised System of Classification and Labelling of Chemicals (GHS) (United Nations, 2009).

7.2.1 Predicted No-Effect Concentration

A PNEC has not been calculated as the notified chemical is not expected to be bioavailable, based on its estimated log K_{ow} of 11.52, and is predicted to have no effect on aquatic biota at its water saturation concentration (ECOSAR (v1.00), US EPA, 2009).

7.3. Environmental risk assessment

A risk quotient (PEC/PNEC) for the notified chemical was not calculated as a PNEC was not derived. However, the notified chemical is likely to have very limited aquatic exposure based on the expected efficient removal of the chemical from waste water by sorption to sewage sludge and biodegradation. The notified chemical is also not expected to be bioavailable to aquatic organisms in surface waters based on its intrinsic hydrophobicity. Therefore, when used as proposed the notified chemical is not expected to pose a risk to the environment.

8. CONCLUSIONS AND REGULATORY OBLIGATIONS

Hazard classification
Based on the available data on analogue chemicals, the notified chemical is not classified as hazardous according to the *Approved Criteria for Classifying Hazardous Substances* (NOHSC, 2004).

Human health risk assessment
Under the conditions of the occupational settings described, the notified chemical is not considered to pose an unacceptable risk to the health of workers.

When used in the proposed manner, the notified chemical is not considered to pose an unacceptable risk to public health.

Environmental risk assessment
On the basis of the reported use pattern, the notified chemical is not expected to pose a risk to the environment.

Recommendations

CONTROL MEASURES
Occupational Health and Safety

- A copy of the MSDS should be easily accessible to employees.
- If products and mixtures containing the notified chemical are classified as hazardous to health in accordance with the *Approved Criteria for Classifying Hazardous Substances* [NOHSC:1008(2004)] workplace practices and control procedures consistent with provisions of State and Territory hazardous substances legislation must be in operation.

Disposal

- The notified chemical should be disposed of to landfill.

Emergency procedures

- Spills or accidental release of the notified chemical should be handled by physical containment, collection and subsequent safe disposal.

Regulatory Obligations

Secondary Notification
This risk assessment is based on the information available at the time of notification. The Director may call for the reassessment of the chemical under secondary notification provisions based on changes in certain circumstances. Under Section 64 of the *Industrial Chemicals (Notification and Assessment) Act (1989)* the notifier, as well as any other importer or manufacturer of the notified chemical, have post-assessment regulatory obligations to notify NICNAS when any of these circumstances change. These obligations apply even when the notified chemical is listed on the Australian Inventory of Chemical Substances (AICS).

Therefore, the Director of NICNAS must be notified in writing within 28 days by the notifier, other importer or manufacturer:

(1) Under Section 64(1) of the Act; if
- the importation volume exceeds one tonne per annum notified chemical; or
- the notified chemical is imported as a raw ingredient; or

or

(2) Under Section 64(2) of the Act; if
- the function or use of the chemical has changed from an ingredient of cosmetic, skin or hair products at > 5%, or is likely to change significantly;
- the chemical has begun to be manufactured in Australia;
- additional information has become available to the person as to an adverse effect of the chemical on occupational health and safety, public health, or the environment.

The Director will then decide whether a reassessment (i.e. a secondary notification and assessment) is required.

Material Safety Data Sheet
The MSDS of the notified chemical (and products containing the notified chemical) provided by the notifier was were reviewed by NICNAS. The accuracy of the information on the MSDS remains the responsibility of the applicant.

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