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NATIONAL INDUSTRIAL CHEMICALS NOTIFICATION AND ASSESSMENT SCHEME (NICNAS)

FULL PUBLIC REPORT

Dodecanoic acid, monoester with 1,2-butanediol (INCI name: Butylene glycol laurate)

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 the Environment, Water, Heritage and the Arts.

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 334-336 Illawarra Road, Marrickville NSW 2204.

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

TABLE OF CONTENTS

FULL PUBLIC REPORT 3
1. APPLICANT AND NOTIFICATION DETAILS 3
2. IDENTITY OF CHEMICAL 3
3. COMPOSITION 3
4. PHYSICAL AND CHEMICAL PROPERTIES 3
5. INTRODUCTION AND USE INFORMATION. 3
6. HUMAN HEALTH IMPLICATIONS 3
7. ENVIRONMENTAL IMPLICATIONS 3
8. CONCLUSIONS AND REGULATORY OBLIGATIONS 3
APPENDIX A: PHYSICAL AND CHEMICAL PROPERTIES 3
APPENDIX B: TOXICOLOGICAL INVESTIGATIONS 3
BIBLIOGRAPHY 3

FULL PUBLIC REPORT

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1. APPLICANT AND NOTIFICATION DETAILS

APPLICANT(S)
Unilever Australia Limited (ABN 66 004 050 828)
20 Cambridge Street
Epping NSW 2121

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 as follows: Boiling Point, Vapour Pressure, Water Solubility, Hydrolysis as a function of pH, Partition Coefficient, Adsorption/Desorption, Dissociation Constant, Flamability Limits, Autoignition Temperature and Explosive Properties.

PREVIOUS NOTIFICATION IN AUSTRALIA BY APPLICANT(S)
None

NOTIFICATION IN OTHER COUNTRIES
None

2. IDENTITY OF CHEMICAL

MARKETING NAME(S)
COMUPOAL BL

CAS NUMBER
32074-61-6

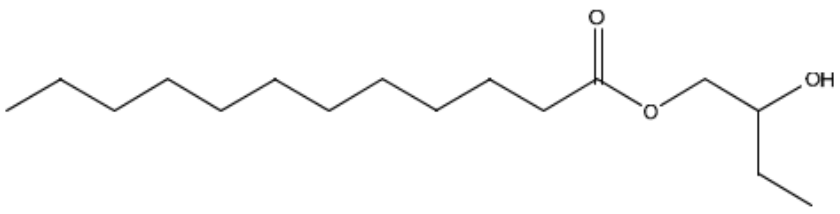
CHEMICAL NAME
Dodecanoic acid, monoester with 1,2-butanediol

OTHER NAME(S)
Butylene glycol laurate (International Nomenclature of Cosmetic Ingredients (INCI) name)
Lauric acid, monoester with 1,2-butanediol
Butylene glycol monolaurate

MOLECULAR FORMULA
$C_{16}H_{32}O_3$

STRUCTURAL FORMULA

Typical structure:



MOLECULAR WEIGHT
272.43 Da

ANALYTICAL DATA
Reference IR information were provided.

3. COMPOSITION

DEGREE OF PURITY Typically 95 - 100%

HAZARDOUS IMPURITIES/RESIDUAL MONOMERS

Chemical Name	Dodecanoic acid		
CAS No.	143-07-7	*Weight %*	Typically < 1.1%
Hazardous properties	R36/38 – Irritating to eyes and skin		

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

Chemical Name	1,3-Butanediol		
CAS No.	107-88-0	*Weight %*	Typically < 4%

Chemical Name	Water		
CAS No.	7732-18-5	*Weight %*	Typically < 0.2%

ADDITIVES/ADJUVANTS None

4. PHYSICAL AND CHEMICAL PROPERTIES

APPEARANCE AT 20°C AND 101.3 kPa: Pale to light yellow liquid

Property	Value	Data Source/Justification
Freezing Point	~2°C	Measured (test report not provided)
Boiling Point	~347°C	Estimated using MPBVP (v1.43)
Density	920 kg/m^3 at 40°C	MSDS
Vapour Pressure	2 x 10^{-7} kPa at 25°C	Estimated using MPBVP (v1.43)
Water Solubility	2.0 x 10^{-3} g/L at 25°C	Estimated using WSKOW (v1.41)
Hydrolysis as a Function of pH	Not determined	The notified chemical is expected to hydrolyse very slowly in the environmental pH range (4–9) at ambient temperature
Partition Coefficient (n-octanol/water)	log K_{ow} = 5.22	Estimated using KOWWIN (v1.67)
Adsorption/Desorption	log K_{oc} = 3.34	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
Flash Point	176°C	MSDS (Cleveland open cup)
Autoignition Temperature	> 176°C	Based on flash point.
Explosive Properties	Not determined	Does not contain known explosophores

DISCUSSION OF PROPERTIES
For full details of tests on physical and chemical properties, refer to Appendix A.

Reactivity
Stable under normal conditions of use. A maximum shelf life of six months is recommended for the notified chemical.

The notified chemical is not classified as a flammable liquid based on its flash point (NTC, 2007), however it is classified as a C2 combustible liquid (NOHSC 2001).

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 does 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 either as a component of finished cosmetic products (concentrations up to 10%) or neat for local blending into cosmetic products.

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 MANUFACTURER/RECIPIENTS
Unilever Australia Ltd

TRANSPORTATION AND PACKAGING
When imported neat, the notified chemical is expected to be contained within 15 kg drums. Finished cosmetic products containing the notified chemical will typically be imported in 200 mL bottles or 200 g tubes packaged in cardboard cartons. The cartons will be transported by road to the notifier's warehouse and subsequently to retail chains for distribution.

USE
The notified chemical is proposed to be used as a component of rinse off (up to 10%) and leave on (up to 2%) cosmetic products. Such products may include make up removers, foundations, skin cleansers, moisturisers, secondary sunscreens, mascara, lipsticks, shampoos, and conditioners.

OPERATION DESCRIPTION
The notified chemical (neat concentration) will be quality control tested, subsequently manually weighed into a container and transferred into a mixing vessel where it will be blended with other ingredients whilst closed. The resulting blend (containing the notified chemical at concentrations up to 10%) will then undergo further quality testing. The finished product will then be filled into retail containers using an automated filling machine.

The finished products containing the notified chemical will be used by consumers and professionals such as hairdressers or workers in beauty salons. Depending on the nature of the product these could be applied a number of ways such as by hand, using an applicator or sprayed.

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
QC personnel	1	3	12
Reformulation workers	1	8	12
Packaging workers	2	8	12
Store persons	2	4	12

EXPOSURE DETAILS

Reformulation

Dermal, ocular and inhalation (aerosol) exposure of workers to the notified chemical at 100% concentration may occur during opening of the import containers, weighing and transferring the notified chemical into a mixing vessel, and connecting and disconnecting transfer and filling lines. Dermal, ocular and inhalation exposure may also occur to concentrations of up to 10% of the notified chemical during quality control operations, and dispensing of the reformulated product into end use containers. Exposure is expected to be lowered by the enclosed nature of the mixing vessel, the automated systems used for mixing and dispensing, the use of exhaust hoods, and workers wearing of personal protective equipment (PPE), such as overalls, face-mask or safety glasses, safety shoes, gloves and respiratory protection (if ventilation is inadequate).

End-Use

Dermal, ocular, and inhalation exposure to the notified chemical at concentrations up to 10% may occur in professions where the services provided involve the application of personal care products to clients (e.g. hair dressers, workers in beauty salons). Such professionals may use some personal protective equipment to minimise repeated exposure, and good hygiene practices are expected to be in place. Exposure of such workers is expected to be of either a similar or higher level than that experienced by consumers using products containing the notified chemical.

6.1.2. Public exposure

Public exposure to the notified chemical is expected to be widespread and frequent through daily use of personal care products containing the notified chemical at concentrations up to 10%. The principal route of exposure will be dermal, while ocular and inhalation exposure is also possible, particularly if products are applied by spray. Exposure to the notified chemical will vary depending on individual use patterns. Data on typical use patterns of a number of product categories in which the notified chemical is proposed to be used are shown below (European Commission 2003, SCCP 2006, Loretz et al 2008). For the purposes of the exposure assessment, Australian use patterns for the various product categories are assumed to be similar to those in Europe.

Considering the physicochemical data that is available for the notified chemical (log K_{ow} = 5.22 and water solubility 2 x 10^{-3} g/L), the default dermal absorption of 100% was assumed for calculation purposes (European Commission, 2003). The actual level of dermal absorption may be lower than 100%. An adult bodyweight of 60 kg has been used for calculation purposes.

Product type	mg/event	events/day	C (%)	RF	Daily exposure (mg/day)	$D_{int,derm}$ (mg/kg bw/day)
Leave on						
Body lotion	8000	1	2	1	160	2.67
Eye and face make up*	110	1- 2 (1.5 used for calcs)	2	1	3.3	0.055
Face cream	1540	2	2	1	61.6	1.03
Lipstick	57	4	2	1	4.56	0.076
General purpose cream	1200	2	2	1	48	0.8
Rinse off						
Bath products	17000	0.29	10	0.001	0.49	0.008
Facial cleansers	4060	1-2 (1 used for calcs)	10	0.01	4.06	0.07
Facial masks	3700	0.1	10	0.1	3.70	0.06
Make up remover	2500	1	10	0.1	25.00	0.42
Shower gel	5000	1.07	10	0.01	5.35	0.089
Shampoo	10460	1	10	0.01	10.46	0.1743
Hair conditioner	14000	0.28	10	0.01	3.92	0.0653
TOTAL						**5.52**

* Sum of five different products: eye shadow; mascara; eyeliner; eyebrow pencil; and concealer

The worst case scenario estimation using these assumptions is for a person who is a simultaneous user of all products listed in the above table. This would result in a combined internal dose from dermal exposure of 5.52 mg/kg bw/day.

6.2. Human health effects assessment

The results from toxicological investigations conducted on the notified chemical are summarised in the table below. Details of these studies can be found in Appendix B.

Endpoint	*Result and Assessment Conclusion*
Rat, acute oral toxicity	Low oral toxicity (LD50 > 2500 mg/kg bw)
Rabbit, skin irritation (10%)	slightly irritating
Rabbit, skin irritation (100%)	slightly irritating
Rabbit, eye irritation	slightly irritating
Guinea pig, skin sensitisation – adjuvant test	no evidence of sensitisation
Mutagenicity – bacterial reverse mutation	non mutagenic

Toxicokinetics
Dermal absorption of the notified chemical may occur but would be limited to some extent by the relatively high log K_{ow} (estimated to be 5.22). However the notified chemical is expected to have surfactant properties, which would enhance its dermal uptake and that of other compounds.

Inhalation of aerosols containing the notified chemical may result in uptake to the respiratory tract.

Metabolites of the notified chemical may include the constituents of the ester, butane diol and lauric acid.

Acute toxicity
The notified chemical was found to be of low acute oral toxicity (LD50 > 2500 mg/kg bw). No acute toxicity data is available on dermal or inhalation toxicity of the notified chemical.

Irritation and Sensitisation
The skin irritation of the notified chemical was tested separately at concentrations of 10% and 100% using an in-house method of the test laboratory. Some irritation was observed in the tests conducted at both concentrations. These results suggest that the notified chemical is likely to be a slight skin irritant, though noting that the test

methods did not enable classification according to the *Approved Criteria for Classifying Hazardous Substances* (NOHSC, 2004). A human patch test using the notified chemical was also performed on 35 subjects. Under the conditions of the test, no signs of skin irritation were observed in any of the subjects.

The notified chemical was found to be slightly irritating to the eyes in a rabbit study.

Using a Magnusson-Kligman guinea pig maximisation test, there was no evidence of reactions indicative of skin sensitisation to the notified chemical.

Mutagenicity
The notified chemical was found to be non-mutagenic in a bacterial reverse mutation assay.

No repeat dose toxicity data are provided to calculate the margin of exposure (MoE) during repeated use of cosmetics containing the notified chemical. A 42-day repeat dose oral toxicity study with the potential metabolite, 1,2-butanediol, established a NOEL of 200 mg/kg bw/day in rats based on transient hypolocomotion (behavioural alterations) and hypopnea (reduced breathing) observed in females at the next dosage level of 1000 mg/kg bw/day (OECD, 1995). No effects are reported in males at 200 or 1000 mg/kg bw/day.

A structurally related group of chemicals (coconut oil and coconut derivatives) has been the subject of a Cosmetic Ingredient Review (CIR, 2008). The review reports the low toxicity of coconut oil, coconut acid, hydrogenated coconut oil and hydrogenated coconut acid.

Health hazard classification
Based on the available data 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
Dermal, ocular and inhalation exposure of workers to the notified chemical at up to 100% concentration may occur during formulation of cosmetics. At such concentrations there is a possibility of slight skin and/or eye irritancy effects. However, given the measures in place to lower exposure, the risk of irritancy is not considered to be unacceptable.

The risk for beauty care professionals who regularly use products containing the notified chemical (up to 10%) is expected to be of a similar or perhaps higher level than that experienced by members of the public who use such products on a regular basis. This is because the duration of exposure will be longer for workers applying products in many clients. No repeat dose toxicity studies were conducted on the notified chemical. The risk of toxicity following repeated exposure is described below under public health.

6.3.2. Public health
At the proposed use concentration of up to 10% or up to 2%, skin or eye irritation is not expected; additionally, the rinse off nature of the products containing the notified chemical at 10% concentration and corresponding relatively short skin contact times are likely to further reduce the potential for irritancy effects.

An estimate of the MoE of the notified chemical was calculated for both rinse-off and leave-on products using the worst case scenarios, as estimated in the table of Section 6.1.2, and the NOEL of 200 mg/kg bw/day for the potential metabolite, 1,2-butanediol. Using the total systemic dose calculated in Section 6.1.2 (5.52 mg/kg bw/day), the MoE is not acceptable (<100) for combined use of all possible products containing the notified chemical. However, this is not expected under normal use situations. MoE greater than or equal to 100 are considered acceptable to account for intra- and inter-species differences. The MoE estimates are shown in the following table:

Product Type	Concentration	Product Giving the Highest Exposure Value	$D_{int,derm}$ (mg/kg bw/day)	MoE
Rinse-off	10%	Make-up remover	0.42	476
Leave-on	2%	Body lotion	2.67	75
Leave-on	2%	Body lotion	2.67	100*

*Calculation of an acceptable MoE value (≥100) requires a NOEL of 267.

The above estimates show that the use of the notified chemical in rinse-off products at up to 10% is acceptable (MoE ≥100). Using the NOEL of 200 mg/kg bw/day established for a potential metabolite, the MoE is not acceptable (MoE <100) for leave-on products containing the notified chemical at 2% (MoE = 75). However, the NOEL used in the estimation of the MoE was based on transient behavioural alterations and breathing difficulties seen at 1000 mg/kg bw/day in females. Considering the gap between the 2 doses tested in the study (200 and 1000 mg/kg bw/day) and due to the transient and mild nature of the effects seen at 1000 mg/kg bw/day, using 200 mg/kg bw/day may have over-estimated the risk. As shown in the table above, a NOEL of 267 mg/kg bw/day would have estimated an acceptable MoE (≥100). Therefore, the use of the notified chemical at 2% in leave-on products is not considered to be unacceptable.

In summary, based on the available data, the notified chemical is not considered to pose an unacceptable risk to public health at concentrations up to 10% in rinse-off cosmetic products and up to 2% in leave-on 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 and will also be imported neat for blending. The notified chemical is expected to be released to landfill as residue in containers (estimated to be up to 1% of the annual import volume) and released to sewer from the cleaning of blending equipment (up to 3%).

Accidental spills during transport or reformulation 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} (3.34). Although the notified chemical has a moderate molecular weight and a high calculated log K_{ow} (5.2), calculations with BCFBAF (v3.00) (US EPA, 2009) indicate a low bioconcentration potential (BCF = 54.5 L/kg wet-wt). Notified chemical in sludge or landfill is expected to degrade through biotic and abiotic processes to form water and oxides of carbon.

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 the notified chemical from influent by sewage treatment plant (STP) processes is expected. 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.

7.2. Environmental effects assessment

No experimental ecotoxicological data were submitted. Modelled estimates (ECOSAR (v1.00); esters SAR) were provided by the notifier, which indicated that the notified chemical is very toxic to all three aquatic trophic levels. However, as the log K_{ow} of the notified chemical is >5, the neutral organics structure-activity relationship (SAR) should be used to estimate endpoints (Clements, 1996). The modelled estimates (ECOSAR (v1.00), neutral organics SAR; US EPA, 2009) of the notified chemical are tabulated below.

Endpoint	*Predicted Result*	*Assessment Conclusion*
Acute toxicity		
Fish	LC50 (14 d) = 0.329 mg/L	Very toxic to fish
Daphnia	LC50 (48 h) = 0.280 mg/L*	Not harmful to aquatic invertebrates at saturation*
Algae	EC50 (96 h) = 0.538 mg/L	Very toxic to algae
Chronic toxicity		
Fish	ChV‡ (30 d) = 0.040 mg/L	Toxic to fish with long lasting effects
Daphnia	ChV‡ (16 d) = 0.054 mg/L	Toxic to aquatic invertebrates with long lasting effects
Algae	ChV‡ = 0.352 mg/L	Harmful to algae with long lasting effects

* If the log K_{ow} is >5 then no effects at saturation are predicted in acute toxicity tests
‡ ChV (Chronic Value) = $(LOEC \times NOEC)^{½}$

Under the Globally Harmonised System of Classification and Labelling of Chemicals (GHS) (United Nations, 2009) the notified chemical is considered to be very acutely toxic to fish and algae, however there are predicted to be 'no effects at saturation' for daphnid acute toxicity.

The notified chemical is classified as chronically toxic with long lasting effects to fish and aquatic invertebrates and is classified as harmful with long lasting effects to algae. The long-term hazard classifications for the notified chemical were determined by comparison of the calculated chronic values (ChV = $(LOEC \times NOEC)^{½}$) and the limiting NOEC values defined for each classification. For example, the 30 d ChV for fish is estimated to be 0.040 mg/L and the $NOEC_{fish}$ must therefore be <0.040 mg/L. As the $NOEC_{fish}$ is less than the NOEC defined as Chronic Category 2 (≤ 0.1 mg/L) the notified chemical is classified as chronically toxic with long lasting effects to fish.

7.2.1 Predicted No-Effect Concentration

The predicted no-effect concentration (PNEC) has been calculated from the estimated 14 day acute fish toxicity of the notified chemical and an assessment factor of 100, as endpoints for three trophic levels were reliably estimated by the neutral organics SAR (ECOSAR (v1.00); US EPA, 2009). Whilst the acute endpoint for daphnia was the lowest predicted endpoint, it was not used in the calculation of the PNEC as the SAR model limitations indicate that there are 'no effects at saturation' when the log K_{ow} is >5.

Predicted No-Effect Concentration (PNEC) for the Aquatic Compartment		
LC50 (Fish)	0.33	mg/L
Assessment Factor	100	
PNEC:	3.29	µg/L

7.3. Environmental risk assessment

Based on the above PEC and PNEC values, the following Risk Quotient (Q) has been calculated:

Risk Assessment	*PEC µg/L*	*PNEC µg/L*	*Q*
Q - River:	0.65	3.29	0.197
Q - Ocean:	0.06	3.29	0.020

The risk quotient for discharge of treated effluents containing the notified chemical to riverine environments is relatively narrow as a result of the estimated high toxicity of this chemical. However, the SimpleTreat Model (European Commission, 2003) estimates that up to 82% of the quantity of the notified chemical being disposed to sewer may be removed in the sewage treatment plant (31% degradation and 51% partitioning to sludge). In this scenario the PEC_{river} is calculated to be 0.12 µg/L and the Q_{river} = 0.035. As the risk quotients have been demonstrated to be <1, the notified chemical is not expected to pose a risk to the environment based on the reported use in cosmetics and the maximum annual importation volume.

8. CONCLUSIONS AND REGULATORY OBLIGATIONS

Hazard classification

Based on the available data the notified chemical is not classified as hazardous according to the *Approved Criteria for Classifying Hazardous Substances* [NOHSC:1008(2004)].

The classification of the notified chemical using the Globally Harmonised System for the Classification and Labelling of Chemicals (GHS) (United Nations 2003) is presented below. This system is not mandated in Australia and carries no legal status but is presented for information purposes.

	Hazard category	*Hazard statement*
Aquatic environment	Acute Category 1	Very toxic to aquatic life
	Chronic Category 2	Toxic to aquatic life with long lasting effects

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 calculated PEC/PNEC ratio and the reported use pattern, the notified chemical is not expected to pose a risk to the environment.

Recommendations

CONTROL MEASURES
Occupational Health and Safety

- Employers should implement the following safe work practices to minimise occupational exposure during handling of the notified chemical at 100% concentration:
  - Avoid skin and eye contact

- Employers should ensure that the following personal protective equipment is used by workers to minimise occupational exposure to the notified chemical (at 100% and up to 10% in cosmetics):
  - Gloves, overalls.

  Guidance in selection of personal protective equipment can be obtained from Australian, Australian/New Zealand or other approved standards.

- 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;

- the notified chemical is to be used in leave-on cosmetic products at concentrations >2% and/or in rinse-off cosmetic products at >10%.

or

(2) Under Section 64(2) of the Act; if

- the function or use of the chemical has changed from a component of rinse off and leave-on cosmetic products;
- the amount of chemical being introduced has increased from 1 tonne per annum, or is likely to increase, 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 provided by the notifier was reviewed by NICNAS. The accuracy of the information on the MSDS remains the responsibility of the applicant.

APPENDIX A: PHYSICAL AND CHEMICAL PROPERTIES

Water Solubility 2.0×10^{-3} g/L at 25°C

Method In house method.
Remarks Flask Method. Three samples of the notified chemical (5 g, 0.5 g and 0.03 g) were each added to a beaker of water (1.0 L) at 22 °C. The beakers were vigorously stirred (15 min) and left to stand. After 24 h, clear oil-like droplets were observed to be floating on the water surface. It was reportedly not feasible to accurately test solubility at lower concentrations, thus the water solubility was reported as <30 mg/L.
The water solubility was estimated to be 2.0×10^{-3} g/L at 25°C (WSKOW (v1.41)), calculation based on the estimated log K_{ow} value 5.22 (KOWWIN (v1.67)) (US EPA, 2009). The notified chemical is expected to have low water solubility based on its predominantly hydrophobic structure.
Test Facility Unilever (2010)

Hydrolysis as a Function of pH Not determined

Remarks The notified chemical contains ester functionality, but has low solubility in water. Therefore, it is expected to hydrolyse very slowly in the environmental pH range (4–9) at ambient temperature.

Partition Coefficient (n-octanol/water) log K_{ow} = 5.22

Method KOWWIN (v1.67) (US EPA, 2009)
Remarks The partition coefficient for the notified chemical was estimated using the QSAR estimations program KOWWIN (v1.67). The notified chemical is expected to partition from water to octanol based on its predominantly hydrophobic structure.
Test Facility US EPA (2009)

Adsorption/Desorption log K_{oc} = 3.34

Method KOCWIN (v2.00) (US EPA, 2009)
Remarks The adsorption coefficient for the notified chemical was estimated using the QSAR estimations program KOCWIN (v2.00). The notified chemical is expected to partition to organic matter in soil and sewage sludge from water based on its predominantly hydrophobic structure.
Test Facility US EPA (2009)

APPENDIX B: TOXICOLOGICAL INVESTIGATIONS

B.1. Acute toxicity – oral

TEST SUBSTANCE	Notified chemical
METHOD	OECD TG 423 Acute Oral Toxicity – Acute Toxic Class Method. EC Directive 92/69/EEC B.1tris Acute Oral Toxicity – Acute Toxic Class Method.
Species/Strain	Rat / Sprague-Dawley CD (Crl:CD (SD) IGS BR) Strain
Vehicle	None
Number of Animals	3 males, 3 females
Remarks - Method	No significant protocol deviations
RESULTS	
Remarks - Results	There were no mortalities observed. Based on the decision tree in the test method, the LD50 can be considered to be >2500 mg/kg bw.
LD50	> 2500 mg/kg bw
Signs of Toxicity	None
Effects in Organs	None
CONCLUSION	The notified chemical is of low toxicity via the oral route.
TEST FACILITY	SafePharm (2001a)

B.2. Irritation – skin

TEST SUBSTANCE	Notified chemical (10%)
METHOD	In-house method
Species/Strain	Rabbit/Japanese White
Number of Animals	3 females
Vehicle	Liquid paraffin
Observation Period	48 hours after patch removal
Type of Dressing	Occlusive
Remarks - Method	Application sites: 4 sites of abraded skin (dermis undamaged) and 4 sites of normal skin. 0.5 mL of the test substance solution was placed on cotton lint with adhesive plaster and applied to previously clipped area of skin. The area was covered with a spongy adhesive cover and a stretchable adhesive sheet and left for 24 hours. Skin irritation was assessed according to the Draize scale at 3, 24, and 48 hours after the patch removed. A positive control was not included in the test.
RESULTS	
Remarks - Results	Irritation was observed at the damaged sites of two of the animals. Well-defined erythema was noted in both animals at the 3 hour observation. In one animal, this remained at the final 48 hour observation, whilst in the other, it had cleared by 48 hours. There were no signs of irritation on any of the normal skin sites.
CONCLUSION	The test substance is slightly irritating to the skin.
TEST FACILITY	Saitama (2001a)

B.3. Irritation – skin

TEST SUBSTANCE	Notified chemical

METHOD
- Species/Strain: Rabbit/Japanese White
- Number of Animals: 3 females
- Vehicle: None
- Observation Period: 48 hours after patch removal
- Type of Dressing: Occlusive
- Remarks - Method: Application sites: 4 sites of abraded skin (dermis undamaged) and 4 sites of normal skin.
0.5 mL of the test substance solution was placed on cotton lint with adhesive plaster and applied to previously clipped area of skin. The area was covered with a spongy adhesive cover and a stretchable adhesive sheet and left for 24 hours. Skin irritation was assessed according to the Draize scale at 3, 24, and 48 hours after the patch removed. A positive control was not included in the test.

RESULTS
- Remarks - Results: Very slight erythema was observed at normal skin sites in all animals, 3 hours after patch removal. This disappeared 24 hours after patch removal. Well defined erythema was observed at damaged skin sites in 2 animals, 3 hours after patch removal. The erythema disappeared in one animal but remained in the other by 48 hours.

CONCLUSION: The notified chemical is slightly irritating to the skin.

TEST FACILITY: Saitama (2001b)

B.4. Irritation – eye

TEST SUBSTANCE: Notified chemical

METHOD
- Species/Strain: Rabbit/Japanese White
- Number of Animals: 3 females
- Observation Period: 72 hours
- Remarks - Method: Eyes were examined 1, 3, 6, 24, 48, and 72 hours following administration. An examination with fluorescein staining was carried out at 24 h.

RESULTS

Lesion	*Mean Score* Animal No.*			*Maximum Value*	*Maximum Duration of Any Effect*	*Maximum Value at End of Observation Period*
	1	2	3			
Conjunctiva: redness	0	0	0	1	< 24 hr	0
Conjunctiva: chemosis	0	0	0	1	< 6 hr	0
Conjunctiva: discharge	0	0	0	2	< 3 hr	0
Corneal opacity	0	0	0	0	-	0
Iridial inflammation	0	0	0	0	-	0

*Calculated on the basis of the scores at 24, 48, and 72 hours for EACH animal.

- Remarks - Results: Conjunctival hyperaemia, edema and discharge were observed, all of which had resolved completely by 24 hours.

CONCLUSION: The notified chemical is slightly irritating to the eye.

TEST FACILITY: Saitama (2001c)

B.5. Skin sensitisation

TEST SUBSTANCE	Notified chemical
METHOD	Similar to OECD TG 406 Skin Sensitisation – Magnusson and Kligman guinea pig maximisation test.
Species/Strain	Guinea pig/Hartley
PRELIMINARY STUDY	Maximum Non-irritating Concentration (at 72 hour observation): intradermal: 3% topical: 10%
MAIN STUDY	
Number of Animals	Test Group: 10 Control Group: 5
INDUCTION PHASE	Induction Concentration: intradermal: 10% topical: 30%
Signs of Irritation	Observation was not recorded in the test report.
CHALLENGE PHASE	
1st challenge	topical: 10%, 3%
Remarks - Method	No significant protocol deviations. vehicle: liquid parrafin

RESULTS

Animal	*Challenge Concentration*	*Number of Animals Showing Skin Reactions after: 1st challenge*	
		24 h	*48 h*
Test Group	10%	2/10	3/10
	3%	0/10	0/10
Control Group	0%	1/5	1/5

Remarks - Results	The skin reactions observed in challenge animals (as tabulated above) were only of mild/scattered redness, including in the control groups.
CONCLUSION	There was no evidence of reactions indicative of skin sensitisation to the notified chemical under the conditions of the test.
TEST FACILITY	Saitama (2001d)

B.6. Genotoxicity – bacteria

TEST SUBSTANCE	Notified chemical
METHOD	OECD TG 471 Bacterial Reverse Mutation Test. EC Directive 2000/32/EC B.13/14 Mutagenicity – Reverse Mutation Test using Bacteria. Plate incorporation procedure
Species/Strain	*S. typhimurium*: TA1535, TA1537, TA98, TA100 *E. coli*: WP2uvrA
Metabolic Activation System	S9 fraction from rat liver induced with phenobarbitone/β-naphthoflavone
Concentration Range in Main Test	a) With metabolic activation: 15 – 5000 µg/plate b) Without metabolic activation: 0.5 - 5000 µg/plate
Vehicle	Acetone
Remarks - Method	No significant protocol deviations. The preliminary study was performed using TA100 and WP2uvrA tester strains. An additional concentration level was included in Test 2, to ensure that there was a minimum of four non-toxic doses.

RESULTS

Metabolic Activation	*Test Substance Concentration (μg/plate) Resulting in:*			
	Cytotoxicity in Preliminary Test	*Cytotoxicity in Main Test*	*Precipitation*	*Genotoxic Effect*
Absent				
Test 1	≥ 150	≥ 50	≥ 5000	Negative
Test 2	-	≥ 50	≥ 5000	Negative
Present				
Test 1	≥ 1500	≥ 1500	≥ 5000	Negative
Test 2	-	≥ 1500	≥ 5000	Negative

Remarks - Results: The test substance did not cause a marked increase in the frequency of revertants per plate of any of the tester strains either in the presence or absence of metabolic activation. Negative controls were within historical limits. Positive controls confirmed the sensitivity of the test system.

CONCLUSION: The notified chemical was not mutagenic to bacteria under the conditions of the test.

TEST FACILITY: SafePharm (2001b)

B.7. Skin irritation – human skin patch test

TEST SUBSTANCE: Notified chemical (30% concentration)

METHOD

Study Group: 35 subjects: 18 men, 17 women (aged 18 – 65)

Vehicle: Petrolatum

Remarks - Method: The test substance (0.01g) was applied in a Finn chamber to a flexor of the upper arm under an occlusive patch for 24 hours. The applied sample was removed 24 hours after application, and effects of the sample were assessed by examining the skin condition 1 hour and 24 hours after sample removal.
The test was carried out during summer.

RESULTS

Remarks - Results: All subjects completed the test. No skin reactions were noted in any subject at the observation times.

CONCLUSION: A human skin patch test was conducted using notified chemical diluted with petrolatum to 30% under occlusive dressing. The notified chemical was non-irritating under the conditions of the test.

TEST FACILITY: Japan Hair Science Association (2001)

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