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NATIONAL INDUSTRIAL CHEMICALS NOTIFICATION AND ASSESSMENT SCHEME (NICNAS)

FULL PUBLIC REPORT

Acetic acid, phenoxy-, 2-hydroxyethyl ester

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Director
Chemicals Notification and Assessment

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1. APPLICANT AND NOTIFICATION DETAILS

APPLICANT(S)
International Flavours and Fragrances Australia Ltd.
301 Frankston-Dandenong Road
Dandenong South
Victoria 3175

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)
No variation to the schedule of data requirements is claimed.

PREVIOUS NOTIFICATION IN AUSTRALIA BY APPLICANT(S)
None

NOTIFICATION IN OTHER COUNTRIES
Phillippines (low volume).

2. IDENTITY OF CHEMICAL

CHEMICAL NAME
Acetic acid, phenoxy-, 2-hydroxyethyl ester

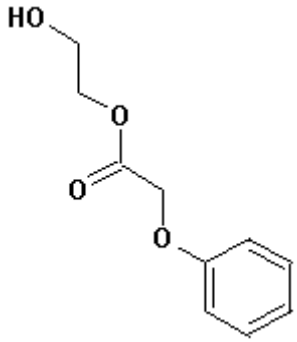
OTHER NAME(S)
Ethylene glycol, phenoxyacetate
2-Hydroxyethyl phenoxyacetate

MARKETING NAME(S)
Veilex #5

CAS NUMBER
1984-60-7

MOLECULAR FORMULA
$C_{10}H_{12}O_4$

STRUCTURAL FORMULA



MOLECULAR WEIGHT
196.2

SPECTRAL DATA

METHOD	UV, using neutral, acidic and basic aqueous solutions Concentrations used ranged from 7.87 x 10^{-4} M to 5.85 x 10^{-5} M
Remarks	A broad absorbance range of 200-225 nm was observed at all three pH values tested. Interpretation of the spectra and calculation of the Emax (ε) values was complicated by uncertainty about which peaks were attributable to the notified chemical and which to the dimer impurity.
TEST FACILITY	IFF (2003)

METHOD	NMR spectrum
Remarks	^{1}H, 7.30, 7.00, 6.92, 4.68, 4.61, 4.43, 4.33, 3.82, 1.91 ppm Solvent used was deuterated chloroform. Spectrum indicates >90% of the notified chemical is present, and < 10% of the dimer impurity. This suggests higher purity than results from the GC analysis.
TEST FACILITY	IFF (2003)

METHOD	IR
Remarks	3496, 2991, 2919, 1767, 1734, 1595, 1496, 1436, 1403, 1297, 1217, 1088, 893, 750 cm^{-1}. Peaks are consistent with the known structure.
TEST FACILITY	IFF (2003)

METHOD	Mass spectrum
Remarks	Electron Impact ionisation A total ion chromatogram was provided, showing two main peaks.
TEST FACILITY	IFF (2003)

METHODS OF DETECTION AND DETERMINATION

METHOD	GC and GC/MS total ion chromatogram
Remarks	FID detector for GC analysis, OV1 and CBW columns. IE value (CBW/OV1): 20.94/11.67 and 20.26 Area percentages of 49.95 and 47.99% (OV1) for the notified chemical and dimer impurity respectively in the GC suggest an approximate 1:1 ratio for these two chemicals. A GC/MS total ion chromatogram confirmed that there are two major components. The ratio obtained from the GC analysis differs from that obtained in the NMR spectrum, where the notified chemical was the major constituent of the mixture. The analytical report suggests that due to the difficulty of obtaining a representative sample of the solid and the small sample size, the samples used in the two tests may have varied.
TEST FACILITY	IFF (2003)

3. COMPOSITION

DEGREE OF PURITY
91% typical, 90-93% range.

HAZARDOUS IMPURITIES/RESIDUAL MONOMERS
None identified

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

Chemical Name	Acetic acid, phenoxy-, 1,2-ethanediyl ester		
CAS No.	85708-29-8	*Weight %*	8% typical* 7-9% range

* Some analytical results indicated a significantly higher proportion of this impurity, comparable to that of the notified chemical

ADDITIVES/ADJUVANTS

Chemical Name	Phenol, 2,6-bis(1,1-dimethylethyl)-4-methyl-		
CAS No.	128-37-0	*Weight %*	0.1 – 0.3%

4. INTRODUCTION AND USE INFORMATION

MODE OF INTRODUCTION OF NOTIFIED CHEMICAL (100%) OVER NEXT 5 YEARS
The notified chemical will be introduced as a component of a fragrance oil or of a consumer product.

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

Year	*1*	*2*	*3*	*4*	*5*
Tonnes	0.2	0.3	0.35	0.4	0.5

USE **Non-Confidential**
Odour masker in household and cosmetic products at a typical concentration of 0.08 – 0.4%. The products will include sun creams, some of which are therapeutic products rather than cosmetics.

5. PROCESS AND RELEASE INFORMATION

5.1. Distribution, transport and storage

PORT OF ENTRY
Sydney

IDENTITY OF MANUFACTURER/RECIPIENTS
International Flavours and Fragrances Australia Ltd.

TRANSPORTATION AND PACKAGING
The notified chemical will be imported into Australia as a component of finished fragrance oils in sealed, polypropylene lined steel drums (55 gallon) or as a component of a finished consumer products in less than 1000 mL containers. When imported as component of a fragrance oil, the notified chemical will be transported from the docks by road to the notifiers warehouse, and then to customers as needed, typically by road.

5.2. Operation description

The notified chemical will be imported as either a component of a finished fragrance oil or end-use consumer product. If imported as a component of an end-use consumer product, no further formulating is required. The product will be sold as imported.

If imported as a component of a finished fragrance oil, the oil will be blended with other ingredients at customer formulation sites, to make end-use consumer products such as sun creams, deodorants, air fresheners, soaps and detergents. While the formulation process will vary with the product type and formulation site, it is expected that most sites will have automated mixing and filling equipment. The

packaged consumer products would be transported to retail outlets for sale to the public.

5.3. Occupational Exposure

Number and Category of Workers

Category of Worker	*Number*	*Exposure Duration*	*Exposure Frequency*
Waterside and transport	4-8	4 hr	4 days/year
Warehouse	2-4	2hr	240 days/year
Mixer	5	4 hr	2 days/year
Quality control worker	2	0.5 hr	2 days/year
Packager	10	4 hr	2 days/year
Maintenance	5	4 hr	2 days/year

Exposure Details

Import and Transport of fragrance oil

The notified chemical will be imported as a component of fragrance oils at up to 8%. These will be transported by road from the docks to the notifier's warehouse, and then distributed to clients for reformulation. Transport and warehouse workers will only be exposed to the notified chemical in the event of container breakage and/or accidental spillage. Workers will wear protective overalls, hard hats, chemical resistant gloves and safety glasses.

Formulation of consumer products

Following distribution to formulators, import containers of fragrance oil containing the notified chemical will be opened and reformulated into consumer products. The major occupational exposure to the notified chemical will be during weighing and addition to the mixing tank. The consumer products manufacturing sites are typically automated. Workers have potential for exposure to the fragrance oil containing up to 8% of the notified chemical and/or the final consumer product containing up to 0.4% of the notified chemical during mixing, packaging, cleaning of equipment and sampling for quality control purposes. The main route of exposure is by skin contact; however, inhalation may occur. Coveralls, gloves and safety glasses are expected to be worn by workers at formulation sites.

Import of consumer products

Where the notified chemical is imported as a component of finished consumer products (at up to 0.4%), worker exposure would occur only in case of accidental breaching of the packaging.

5.4. Release

RELEASE OF CHEMICAL AT SITE

Release to the environment of the notified chemical is not expected to occur at the warehouse site. Potential release could occur from accidents in transportation and from mishandling of containers during manoeuvring operations. Any released notified chemical is expected to be physically contained, collected, and subsequently disposed of to high-temperature incinerator or as trade waste to secure landfill.

Release to the environment of the notified chemical may occur at the reformulation sites, arising from container and equipment rinsing. The quantity of residual notified chemical is not expected to exceed 1% of the total import volume. It is expected that the rinsings, containing the notified chemical will be released to sewer.

RELEASE OF CHEMICAL FROM USE

The notified chemical will be used in household, laundry, and personal cleaning products, with almost all (~97%) of the imported quantity being released to sewer. Approximately 1% of the total imported quantity of the notified chemical is expected to remain as residual in consumer containers, which are primarily disposed of as domestic waste to landfill.

5.5. Disposal

Accidental spills may occur from transport accidents, mishandling of containers, and from reformulation equipment failures. Spills of notified chemical should be contained physically, collected and disposed of by thermal decomposition in high temperature incinerators or sent to secure landfill.

5.6. Public exposure

The main source of public exposure would be through consumer use of household and cosmetic products containing the notified chemical at up to 0.4%. The notified chemical will be used in personal products such as sun creams, deodorants, and soaps, and in household air fresheners.

The notifier has advised that the concentration of the chemical in consumer products will be as follows:

Product category	Percentage in final product
Sun creams / lotions	0.4
Deodorant sprays	0.08
Air freshener sprays	0.12
Soap bars	0.08

For personal products the major route of exposure will be skin contact, however inhalation exposure may also be significant during the application of spray deodorants. Inhalation would be the main route of exposure during use of household air fresheners, especially those designed for spray use .

Inadvertent public exposure to perfume oils containing the notified chemical at up to 8% could occur in case of accidents in transport, however this scenario is not considered likely.

6. PHYSICAL AND CHEMICAL PROPERTIES

Appearance at 20ºC and 101.3 kPa Off white solid

Melting Point 54.6ºC

METHOD EC Directive 92/69/EEC A.1 Melting/Freezing Temperature.
Remarks Differential scanning calorimetry method was used.
TEST FACILITY Safepharm (2003a)

Density 1347 kg/m^3 at 21.5ºC

METHOD EC Directive 92/69/EEC A.3 Relative Density.
Remarks Relative density stated to be 1.35 at 21.5 ± 0.5ºC
TEST FACILITY Safepharm (2003a)

Vapour Pressure 2.2 x 10^{-6} kPa at 25ºC

METHOD EC Directive 92/69/EEC A.4 Vapour Pressure.
Remarks Vapour pressure balance method was used with readings between 31–41%. The correlation between readings was poor however was considered sufficient to assign a value, which rates the notified chemical as slightly volatile (Mensink et al., 1995).
TEST FACILITY Safepharm (2003b)

Water Solubility 12.0 g/L at 20ºC ± 0.5 g/L

METHOD EC Directive 92/69/EEC A.6 Water Solubility (Flask Method).
Remarks A preliminary test was conducted whereby an aliquot (1.5342 g) of test material

was diluted to 100 mL with glass double-distilled water. After shaking at 30ºC for 17 hours and standing at 20ºC for 3 hours, the solution was centrifuged at 13500 rpm for 15 minutes. The supernatant solution still contained excess test material, therefore centrifugation was repeated. The resulting supernatant solution was then taken for analysis.

Based on the preliminary result, mixtures of test material and glass double-distilled water were added to three separate flasks. After addition of glass double-distilled water to the flasks, they were shaken at approximately 30ºC and, after standing at 20ºC for a period of not less than 24 hours, the contents of the flasks were centrifuged as above. The supernatant solution was taken for analysis. The concentration of test material was determined by High Performance Liquid Chromatography (HPLC). The solution pH after 24 hours was 3.1-3.3, ensuring minimal hydrolysis had occurred..

TEST FACILITY Safepharm (2003a)

Hydrolysis as a Function of pH

METHOD EC Directive 92/69/EEC C.7 Degradation: Abiotic Degradation: Hydrolysis as a Function of pH.

pH	*T (°C)*	*$t_{½}$ (Days)*
4	25	>365
7	25	8.51
9	25	<1

Remarks Results from the Preliminary test/Test 1 at 50ºC showed it was necessary to undertake further testing at pH 7, with solutions being maintained at 40.0 ± 0.5ºC for a period of 24 hours.

The kinetics of the study have been determined to be consistent with that of a pseudo-first order reaction as the graphs of log_{10} concentration versus time are straight lines. It has been observed that the rate of hydrolysis increases with an increase in pH. No test material was present at sufficient concentration for detection in the 2.4 hour pH 9 samples. A limit value was therefore quoted, which was taken from the mean area obtained for the lowest concentration linearity standard.

TEST FACILITY Safepharm (2003a)

Partition Coefficient (n-octanol/water) P_{OW} = 6.90 at 20.5 ± 0.5ºC, Log_{10} P_{OW} = 0.839

METHOD EC Directive 92/69/EEC A.8 Partition Coefficient (shake-flask method)

Remarks A preliminary assessment of the partition coefficient was made based on the approximate solubilities of the test material in n-octanol and water. Six partitions were then performed. In each test, the combined value of both phases occupied not less than 90% of the total volume of the test vessel.

The shaking was performed by inversion of the flasks through approximately 180º over a five minute period. After separation, via centrifugation (2900 rpm for 15 minutes), aliquots of both phases were taken for analysis. The concentration of test material in the sample solutions was determined by High Performance Liquid Chromatography (HPLC).

TEST FACILITY Safepharm (2003a)

Adsorption/Desorption – screening test K_{oc} = 13.7, log K_{oc} = 1.14 at 30°C

METHOD EC Directive 2001/59/EC C19 (HPLC Screening Method)

Remarks The notified chemical was compared with 13 reference solutions, and was found to be more mobile than all. Peaks present at approximately 4.6 and 7.9 minutes were

considered to be impurities and therefore were not included in the results.

TEST FACILITY Safepharm (2003a)

Dissociation Constant pKa = 13.84 ± 0.20

METHOD Estimation Software ACD/Chemsketch version 3.50/09 April 1998

Remarks No determination was possible according to OECD 112, as the methods were either not applicable or unsuitable for the determination of the very weak acid. The above has been determined by chemical estimation software.

TEST FACILITY Safepharm (2003a)

Particle Size

METHOD OECD TG 110 Particle Size Distribution/Fibre Length and Diameter Distributions.

Range (μm)	*Mass (%)*
< 100	0.498
≥ 100	99.502

Remarks Test material was sieved for approximately 10 minutes with the aid of a sieve brush through a 100 μm sieve. The mass of the test material passing through the sieve was measured.

TEST FACILITY Safepharm (2003a)

Flash Point 164 °C at 101.32 kPa

METHOD EC Directive 92/69/EEC A.9 Flash Point.

Remarks Closed cup method, usually used for liquids. The solid sample was ground before testing.

TEST FACILITY Safepharm (2003b)

Not highly flammable

METHOD EC Directive 92/69/EEC A.10 Flammability (Solids).

Remarks The test material did not propagate combustion overt he 200 mm of the preliminary screening test. Therefore the main test was not performed.

TEST FACILITY Safepharm (2003b)

Autoignition Temperature > 400°C

METHOD 92/69/EEC A.15 Auto-Ignition Temperature (Liquids and Gases).

Remarks The solid sample was ground before testing. This method is usually applicable to liquids. Temperatures up to 400°C were tested. At 100°C and above, grey fumes were emitted but there was no ignition.

TEST FACILITY Safepharm (2003b)

Explosive Properties Not expected to be explosive.

METHOD EC Directive 92/69/EEC A.14 Explosive Properties.

Remarks Result predicted on basis that there are no chemical groups that would imply explosive properties.

TEST FACILITY Safepharm (2003b)

Reactivity

Remarks The notified chemical is expected to be stable in water and air under normal conditions of temperature and pressure. Carbon monoxide and unidentified organic compounds may be formed during combustion.

Oxidizing Properties Not expected to be oxidising.

METHOD	EC Directive 92/69/EEC A.17 Oxidizing Properties (Solids).
Remarks	Result predicted on the basis that there are no chemical groups that would imply oxidising properties.
TEST FACILITY	Safepharm (2003b)

7. TOXICOLOGICAL INVESTIGATIONS

Endpoint and Result	*Assessment Conclusion*
Rat, acute oral LD50 7,100 mg/kg bw*	low toxicity
Rat, acute dermal LD50 > 7,940 mg/kg bw*	low toxicity
Rabbit, skin irritation*	non-irritating
Rabbit, eye irritation*	slightly irritating
Genotoxicity – bacterial reverse mutation	non mutagenic

* Only abbreviated reports were supplied for these endpoints.

7.1. Acute toxicity – oral

TEST SUBSTANCE — Notified chemical (purity not specified)

METHOD
- Species/Strain: Rat/Sprague-Dawley albino
- Vehicle: 20% suspension in corn oil
- Remarks - Method: Little detail supplied on method.

RESULTS

Group	*Number and Sex of Animals*	*Dose mg/kg bw*	*Mortality*
1	2M, 3F	5,010	1/5 (F)
2	3M, 2F	6,310	1/5 (F)
3	2M, 3F	7,940	4/5 (2M, 2F)
4	3M, 2F	10,000	5/5

- LD50: 7,100 mg/kg bw
- Signs of Toxicity: Increasing weakness and collapse were seen in animals prior to death. Reduced appetite and activity were seen for 1 to 3 days in surviving animals.
- Effects in Organs: Lung and liver hyperemia and gastrointestinal inflammation were observed at autopsy. The dose levels at which these effects occurred was not stated, however the comments may refer to non-surviving animals. The viscera appeared normal at 14 days in surviving animals.
- Remarks - Results: Summary only of results was supplied.

CONCLUSION — The notified chemical is of low toxicity via the oral route.

TEST FACILITY — Younger (1976)

7.2. Acute toxicity – dermal

TEST SUBSTANCE — Notified chemical (purity not specified)

METHOD
- Standard method not specified.
- Species/Strain: Rabbit/New Zealand Albino
- Vehicle: 40% suspension in corn oil
- Type of dressing: Not stated.
- Remarks - Method: Exposure time was 24 h. No further details of the method were provided.

RESULTS

Group	*Number and Sex of Animals*	*Dose mg/kg bw*	*Mortality*
1	1M	5,010	0/1
2	1M, 1F	7,940	0/2

LD50	> 7,940 mg/kg bw
Signs of Toxicity - Local	None reported.
Signs of Toxicity - Systemic	Reduced appetite and activity were observed for 1 to 3 days after testing.
Effects in Organs	Viscera appeared normal after 14 days.
Remarks - Results	No further details were reported.

CONCLUSION The notified chemical is of low toxicity via the dermal route.

TEST FACILITY Younger (1976)

7.4. Irritation – skin

TEST SUBSTANCE Notified chemical (purity not stated)

METHOD	Standard method not specified
Species/Strain	Rabbit/New Zealand Albino
Number of Animals	6
Vehicle	Notified chemical was finely ground and moistened with water.
Observation Period	Seven days.
Type of Dressing	Not stated.
Remarks - Method	Exposure period was 24 h. No further details were provided.

RESULTS

Lesion	*Mean Score**	*Maximum Value*	*Maximum Duration of Any Effect*	*Maximum Value at End of Observation Period*
Erythema/Eschar	0	0	-	0
Oedema	0	0	-	0

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

Remarks - Results No adverse effects were observed.

CONCLUSION The notified chemical non-irritating to the skin.

TEST FACILITY Younger (1976)

7.5. Irritation – eye

TEST SUBSTANCE Notified chemical (purity not stated)

METHOD	Apdaptation of Draize method
Species/Strain	Rabbit/New Zealand White
Number of Animals	6
Observation Period	7 days
Remarks - Method	The notified chemical was finely ground and 0.1 mL (45 mg) was instilled into the conjunctival sac.

RESULTS

Lesion	*Mean Score**	*Maximum Value*	*Maximum Duration of Any Effect*	*Maximum Value at End of Observation Period*
Conjunctivae	N/A	N/A	< 5 days	0
Cornea	N/A	N/A	< 48 h	0
Iris	N/A	N/A	< 48 h	0

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

Remarks - Results Effects on cornea, iris and conjunctivae were rated at 1 h, 24 h, 48 h, 72

h, 5 days and 7 days. The key to the numerical scoring system was not provided. However qualitative descriptions of the effects were given:
10 minutes: Moderate erythema, very slight edema, copious discharge.
1 h: Severe erythema, very slight edema, copious discharge.
24 h: Areas of barely perceptible corneal dullness, iris congestion in two animals, slight to moderate erythema, copious discharge containing whitish exudate.
48 h to 72 h: Gradual improvement.
5 days: All scores zero.

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

TEST FACILITY — Younger (1976)

7.8. Genotoxicity – bacteria

TEST SUBSTANCE — Notified chemical, described as white powder. Purity not specified.

METHOD — Method analogous to OECD TG 471 Bacterial Reverse Mutation Test. Plate incorporation procedure

Species/Strain	*S. typhimurium*: TA1538, TA1535, TA1537, TA98, TA100, *Saccharomyces cerevisiae:* D4
Metabolic Activation System	S9 fraction from Aroclor induced rat liver
Concentration Range in Main Test	a) With metabolic activation: 0.1 to 500 µg/plate b) Without metabolic activation: 0.1 to 500 µg/plate
Vehicle	DMSO
Remarks - Method	No preliminary test was conducted.

RESULTS

Metabolic Activation	*Test Substance Concentration (µg/plate) Resulting in:*			
	Cytotoxicity in Preliminary Test	*Cytotoxicity in Main Test*	*Precipitation*	*Genotoxic Effect*
Absent				
Test 1	N/A	> 500 µg/plate	-	None
Present				
Test 1	N/A	> 500 µg/plate	-	None

Remarks - Results — The test report did not mention whether precipitation occurred, however all plates were able to be scored successfully.
The efficacy of the test system was confirmed by significantly higher numbers of revertants in the positive controls, except for the positive control DMNA (dimethylnitrosamine) used at 100 µmoles/plate with metabolic activation for *Saccharomyces cerevisiae,* D4 strain. In this test the positive control had just under double the revertants of the solvent control. The lower mutagenicity of this positive control under the conditions of the test is likely to result from use of the plate incorporation method, and does not cast doubt on the validity of the test results on the notified chemical. The study authors state that chemicals such as dialkyl nitrosamines are mutagenic in suspension assays but not in the plate assay.

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

TEST FACILITY — Litton Bionetics (1977)

8. ENVIRONMENT

8.1. Environmental fate

No experimental environmental fate or toxicity data were submitted. However, the following data estimated by QSAR were provided based on a predicted water solubility of 5 g/L and log K_{OW} of 0.64.

8.1.1. Ready biodegradability

TEST SUBSTANCE	Notified Chemical
METHOD	BIOWIN Estimation Program v4.00
RESULTS	Linear biodegradation probability = 1.2470 – Biodegrades Fast Non-Linear Biodegradation probability = 0.9999 – Biodegrades Fast *(A probability ≥ 0.5 indicates "Biodegrades Fast".)* Survey Model – Ultimate Biodegradation = 3.0297 – Weeks Survey Model – Primary Degradation = 4.0051 – Days *(≥ 5 → hours; ≥ 4 →Days; ≥ 3 →Weeks; ≥ 2 →Months; ≥ 1 →Longer.)* MITI Linear Biodegradation probability = 1.0179 – Readily Degradable MITI Non-Linear Biodegradation probability = 0.9714 – Readily Degradable *(A probability ≥ 0.5 indicates "Readily Degradable".)*
CONCLUSION	Based on the analysis estimation, the notified chemical is readily degradable, biodegrades quickly with primary biodegradation occurring within days, and ultimate degradation occurring within weeks.
TEST FACILITY	BIOWIN v4.00

8.2. Ecotoxicological investigations

8.2.1. Acute toxicity to fish

TEST SUBSTANCE	Notified Chemical
METHOD	
RESULTS	LC50 158.6 mg/L at 96 hours.
CONCLUSION	The notified chemical has been estimated to be very slightly toxic to fish.
TEST FACILITY	ECOSAR v0.99f

8.2.2. Acute/chronic toxicity to aquatic invertebrates

TEST SUBSTANCE	Notified Chemical
METHOD	
RESULTS	LC50 2693.5 mg/L at 48 hours
CONCLUSION	The notified chemical has been estimated to be very slightly toxic to aquatic invertebrates.
TEST FACILITY	ECOSAR v0.99f

8.2.3. Algal growth inhibition test

TEST SUBSTANCE	Notified Chemical
METHOD	

RESULTS	EC50 12.0 mg/L
CONCLUSION	The notified chemical has been estimated to be harmful to algae.
TEST FACILITY	ECOSAR v0.99f

9. RISK ASSESSMENT

9.1. Environment

9.1.1. Environment – exposure assessment

The notified chemical is imported as part of a finished fragrance oil or final formulated consumer product in sealed containers, which are transported to the notifier's warehouse by road. Potential exposure could arise from drum rupture due to traffic accident or drum mishandling.

From the notifier's warehouse, the import containers are then transported by road to customers as needed. The finished fragrance oil is then incorporated into the final consumer products (sun creams, deodorants, air fresheners and soaps) using largely automated mixing and filling systems. The concentration of the notified chemical in the final consumer products is expected to be less than 0.5%. Environmental exposure is not expected to occur at this stage, as any accidental spills would be contained by standard engineering structures, and after collection, would be disposed either to high-temperature incinerator or as industrial waste to secure landfill. It is expected that less than 1% of the imported quantity of notified chemical will remain as residue in the import containers. The residual chemical is expected to be rinsed, with the rinsings being discharged to sewer. The containers themselves are expected to be disposed of to secure landfill.

Empty consumer product containers, which are expected to be disposed of as domestic waste to landfill, should contain less than 5% of the total imported quantity of notified chemical. The majority of the notified chemical within the final consumer products is expected to be washed off and be discharged to sewer.

Based on maximum annual imports of 500 kg per annum, and assuming a worst-case scenario that all of this is eventually released to sewer and not removed during sewage treatment processes, the daily release on a nationwide basis to receiving waters is estimated to be 1.37 kg/day. Assuming a national population of 20.1 million and that each person contributes 200 L/day to overall sewage flows, the worst-case predicted environmental concentration (PEC) in sewage effluent on a nationwide basis is estimated to be 0.341 µg/L. Based on the respective dilution factors of 1 and 10 for inland and ocean discharges of effluents, the PECs of notified chemical in fresh water and marine will be 0.341 and 0.034 µg/L, respectively.

The SIMPLETREAT model (European Commission, 2003) was used to model the partitioning and losses in sewage treatment plants (STP) throughout Australia. A worst-case scenario was assumed with a very low Henry's Constant (Log H $\leq$ -4) and the log K_{OW} of < 1. The SIMPLETREAT table for chemicals that are readily biodegradable, but do not satisfy the 10-day criterion was used.

The results obtained indicate that when the notified chemical is released into the aqueous phase of a STP, approximately 0% is released to air through volatilisation, 67% is degraded, 33% is partitioned to water, and 0% is partitioned to biosolids. The resulting PECs for the aquatic environment from the nationwide release of the notified chemical into the sewage systems will be less than the above worst case scenario. The PECs from the worst case scenario are used in the following risk assessment.

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/yr). The notified chemical in this volume is assumed to infiltrate and accumulate in the top 0.1 m of soil (density 1000 kg/m^3). Using these assumptions, irrigation with a concentration of 0.341 µg/L may potentially result in a soil concentration of approximately 3.41 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 0.17 and 0.34 mg/kg respectively.

The potential for the notified chemical to bioaccumulate is low due to its relatively high water solubility and will be limited due to the diffused release to sewer Australia wide.

9.1.2. Environment – effects assessment

A Predicted No-Effect Concentration can be calculated, assuming the worst-case scenario data above, and using the lowest EC50 of 12 mg/L (algae), as being 12 µg/L using the safety factor of 1000 (as all toxicity data were estimated using predictive software).

9.1.3. Environment – risk characterisation

The risk quotient (Q) values (PEC/PNEC) for the aquatic environment were determined as follows:

	Worst Case		Mitigated	
Location	PEC µg/L	RQ	PEC µg/L	RQ
Ocean outfall	0.034	0.003	0.011	0.001
Inland River	0.341	0.028	0.112	0.009

Given the diffuse and widespread use of the end-use products, the concentration of the notified chemical in the aquatic compartment is likely to be low. Furthermore, the low Q values indicate that there is unlikely to be an environmental risk to the aquatic compartment.

It is expected that the waste generated during use may be disposed of to landfill. In landfill, residual notified chemical is expected to hydrolyse under alkaline conditions and degrade via biotic processes. Therefore, environmental risk from the reported use pattern of the notified chemical is likely to be low.

Based on the proposed use pattern, the notified chemical is not expected to pose an unacceptable risk to the health of aquatic life. Bioaccumulation is not expected from the diffuse use pattern.

9.2. Human health

9.2.1. Occupational health and safety – exposure assessment

Transport & Storage

Occupational exposure to the notified chemical during transport and storage of imported fragrance oils containing up to 8% the notified chemical is only likely in the event of accidental container breakage and/or spillage. Exposure in these circumstances is expected to be infrequent, and can be limited by use of gloves, goggles, masks and protective clothing during clean-up operations.

Formulation

The formulation and packaging of consumer products containing the notified chemical provides the major potential exposure of workers. During these processes, dermal exposure to the fragrance oil (up to 8% of the notified chemical) or the consumer product (up to 0.4% of the notified chemical) is the most likely route. Ocular exposure may occur due to accidental splashes. The potential for inhalation exposure would be reduced by the low volatility of the notified chemical, which has a vapour pressure of 2.2×10^{-6} kPa at 25°C.

Exposure may occur when workers open the drums of fragrance oil containing imported notified chemical, when weighing and transferring the imported fragrance preparations into mixing vessels, during QC, during blending operations and when cleaning up spills and equipment.

Worker exposure to the notified chemical during filling of consumer product containers is expected to be minimal, as the filling of consumer containers is typically automated and the concentration of notified chemical is lower.

Formulation processes are expected to occur during only 2 days/year at each formulation site, and total forecast usage quantity is ≤ 500 kg/year. Engineering controls, safe work practices and PPE in place at formulation sites would reduce worker exposure.

Overall the exposure to workers is expected to be low because of the intermittent nature of potential exposure, relatively low usage quantities and the controlled nature of the formulation

process.

9.2.2. Public health – exposure assessment

The main source of exposure of the public to the notified chemical would be during consumer use of one or more perfumed end-use household or personal products containing the chemical. There is potential for repeated low-level exposure to the public, through use of products containing the notified chemical.

The greatest potential dermal exposure would occur from body creams deliberately applied to the skin, which are not washed off after use, and contain up to 0.4% of the notified chemical. An example of an above-average use scenario for dermal exposure is as follows:

If it is assumed that skin application of 8 g of a cream occurs 3 times a day, and that there is 100% uptake, (SCCNFP, 2003, Health Canada, 2005) a 60 kg consumer would have dermal exposure to 0.0016 mg/kg bw/day of the notified chemical.

Inhalation exposure can occur during use of both household and personal products, and might be expected to be higher where the product is designed to volatilise quickly eg during use of a spray product. An example of inhalation exposure from spray air freshener containing 0.12% of the notified chemical is as follows:

If it is assumed that 5 g of air freshener is sprayed daily, and there is 100% exposure to and uptake of this quantity, a 60 kg consumer would have inhalation exposure to 0.0001 mg/kg bw/day of the notified chemical.

The above calculations give an indication of possible consumer exposure but would not be representative of the full range of exposure for individuals, which will vary with a number of factors, eg number and type of products used that contain the notified chemical, frequency of use, body weight.

Public exposure from transport, storage, reformulation or disposal is considered to be negligible.

9.2.3. Human health – effects assessment

General
Animal studies on the notified chemical were available for several endpoints, although most tests were carried out more than twenty years ago and do not conform to current testing protocols. Based on recent analytical data, the notified chemical contains a significant proportion of a dimer impurity, which may vary in concentration in the commercial product tested.

No information on toxicokinetics, metabolism and distribution was supplied for the notified chemical. However the partial water solubility (12 g/L) and low partition coefficient (0.839) of the chemical indicate a relatively low potential for crossing biological membranes.

The notifier has stated that the chemical has been in global commerce for more than 25 years, with no known incidence of illness or injury related to it.

Specific endpoints
Based on the study results, the notified chemical is of low oral and dermal toxicity. It is not a skin irritant.

The results of an eye irritation study based on the Draize method suggested that the chemical is a slight eye irritant. Its adverse effects were seen primarily in the conjunctivae, resolving almost completely by 72 h. Corneal and iridial effects were seen at 24 h only. While the scoring system used does not match that in the NOHSC *Approved Criteria for Classifying Hazardous Substances* (NOHSC 2004), the qualitative description of the effects suggests that they would not meet the criteria for classification.

The notified chemical was non-mutagenic in a bacterial reverse mutation study, both with and without metabolic activation.

No information was received on sensitisation potential, repeated dose toxicity, carcinogenicity, or reproductive effects

Based on the available data, the notified chemical is not classified as a hazardous substance in accordance with the NOHSC *Approved Criteria for Classifying Hazardous Substances* (NOHSC 2004).

9.2.4. Occupational health and safety – risk characterisation

On the basis of the data provided, the notified chemical is not acutely toxic by the oral or dermal routes, irritating to skin, or mutagenic to bacteria. The chemical is slightly irritating to eyes, but will not be handled by workers except as part of a mixture (up to 8%) in imported perfume oils, or as part of the finished consumer products (up to 0.4%). At these concentrations the eye irritation effects of the chemical are expected to be low. It should be noted that no data was available for some toxicological endpoints.

Dermal and inhalation exposure to workers may occur during the formulation process, whereby perfume oil is incorporated into consumer products. Inhalation exposure would be reduced by the low volatility of the chemical. Use of engineering controls, safe work practices and PPE would reduce potential exposure. Exposure would be intermittent because formulation would be carried out only occasionally.

Considering that the known toxicity of the notified chemical is low, and expected exposure during formulation is reduced by the factors mentioned above, the risk of adverse effects to workers during formulation is low. During transport and storage of the perfume oils or consumer products, the potential for exposure is very low, and the risk to workers considered similarly very low.

9.2.5. Public health – risk characterisation

The public will be exposed to the notified chemical through use of consumer household and personal care products containing it at levels of 0.08 to 0.4%. Depending on patterns of use, repeated low level dermal and inhalation exposure to consumers may occur. On the basis of the toxicological testing carried out, the notified chemical is of low hazard, however data is not available for several endpoints and a NOAEL has not been determined. An indicative estimate of consumer exposure from end-use of the product category containing the notified chemical at the highest intended concentration (0.4%) is 0.0016 mg/kg bw/day.
Given that the expected exposure via consumer products is low and the known toxicity is low, the chemical is considered to pose a low risk to public health.

10. CONCLUSIONS – ASSESSMENT LEVEL OF CONCERN FOR THE ENVIRONMENT AND HUMANS

10.1. Hazard classification

Based on the available data the notified chemical is not classified as hazardous under the NOHSC *Approved Criteria for Classifying Hazardous Substances*.

and

As a comparison only, the classification of 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.

The notified chemical is not classified for health hazards under the Globally Harmonised System of Classification and Labelling of Chemicals (GHS).

The notified chemical cannot be classified for the environmental hazards under the GHS, as only estimated ecotoxicity data has been provided.

10.2. Environmental risk assessment

On the basis of the PEC_{River}/PNEC ratio of 0.025, the notified chemical is not considered to pose a risk to the environment based on its reported use pattern.

10.3. Human health risk assessment

10.3.1. Occupational health and safety

There is Low Concern to occupational health and safety under the conditions of the occupational settings described.

10.3.2. Public health

There is No Significant Concern to public health when used as planned in consumer household and personal products.

11. MATERIAL SAFETY DATA SHEET

11.1. Material Safety Data Sheet

The MSDS of the notified chemical provided by the notifier was in accordance with the NOHSC *National Code of Practice for the Preparation of Material Safety Data Sheets* (NOHSC 2003). It is published here as a matter of public record. The accuracy of the information on the MSDS remains the responsibility of the applicant.

11.2. Label

The label for the notified chemical provided by the notifier was in accordance with the NOHSC *National Code of Practice for the Labelling of Workplace Substances* (NOHSC 1994). The accuracy of the information on the label remains the responsibility of the applicant.

12. RECOMMENDATIONS

CONTROL MEASURES

Occupational Health and Safety

- Employers should implement the following engineering controls to minimise occupational exposure to the notified chemical in perfume oil blends and consumer products:
  - Use of a closed or semi-closed system for weighing and formulation processes, where possible
  - Local exhaust ventilation or good general ventilation should be provided if the weighing and formulation process is an open one.

- Employers should implement the following safe work practices to minimise occupational exposure during handling of the notified chemical in perfume oil blends and consumer products:
  - Prevent splashes and spills.
  - Avoid direct handling of the perfume blends where possible.

- Employers should ensure that the following personal protective equipment is used by workers to minimise occupational exposure to the notified chemical in perfume oil blends and consumer products:
  - Chemical resistant gloves, protective overalls and goggles/faceshield.

– Respiratory protection should be used if the perfume blend is handled in a confined space.

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 NOHSC *Approved Criteria for Classifying Hazardous Substances*, 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 by thermal decomposition in high-temperature incinerators or to secure landfill.

Emergency procedures

- Spills/release of the notified chemical should be handled by physical containment, collection and disposal of by thermal decomposition in high-temperature incinerators or to secure landfill.

12.1. Secondary notification

The Director of Chemicals Notification and Assessment 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, which will require full results and reports for ecotoxicity testing.

(2) Under Section 64(2) of the Act:
– if any of the circumstances listed in the subsection arise.

The Director will then decide whether secondary notification is required.

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