File No.: LTD/2122

April 2020

NATIONAL INDUSTRIAL CHEMICALS NOTIFICATION AND ASSESSMENT SCHEME (NICNAS)

PUBLIC REPORT

Silicic acid, ethyl 2-phenylethyl ester

This Assessment has been compiled in accordance with the provisions of the *Industrial Chemicals (Notification and Assessment) Act 1989* (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 conducts the risk assessment for public health and occupational health and safety. The assessment of environmental risk is conducted by the Department of Agriculture, Water and the Environment.

This Public Report is 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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SUMMARY

The following details will be published in the NICNAS *Chemical Gazette:*

ASSESSMENT REFERENCE	APPLICANT(S)	CHEMICAL OR TRADE NAME	HAZARDOUS CHEMICAL	INTRODUCTION VOLUME	USE
LTD/2122	Henkel Australia Pty Ltd	Silicic acid, ethyl 2-phenylethyl ester	ND*	< 1 tonne per annum	Fragrance ingredient in household cleaning products

*ND = not determined

CONCLUSIONS AND REGULATORY OBLIGATIONS

Hazard Classification
As only limited toxicity data were provided, the notified chemical cannot be classified according to the *Globally Harmonised System of Classification and Labelling of Chemicals* (GHS), as adopted for industrial chemicals in Australia.

Human Health Risk Assessment
Under the conditions of the occupational settings described, the notified chemical is not considered to pose an unreasonable risk to the health of workers.

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

Environmental Risk Assessment
Based on the low hazard and reported use pattern, the notified chemical is not considered to pose an unreasonable risk to the environment.

Recommendations

CONTROL MEASURES

Occupational Health and Safety

- A person conducting a business or undertaking at a workplace should implement the following engineering controls to minimise occupational exposure to the notified chemical during reformulation:
  - Enclosed/automated processes
  - Local exhaust ventilation

- A person conducting a business or undertaking at a workplace should implement the following safe work practices to minimise occupational exposure during handling of the notified chemical during reformulation:
  - Avoid contact with skin and eyes
  - Avoid inhalation of aerosols
  - Remove all sources of ignition

- A person conducting a business or undertaking at a workplace should ensure that the following personal protective equipment is used by workers to minimise occupational exposure to the notified chemical during reformulation:
  - Protective clothing
  - Impervious gloves
  - Safety glasses or goggles
  - Respiratory protection if inhalation exposure may occur

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

- A copy of the SDS should be easily accessible to employees.

- If products and mixtures containing the notified chemical are classified as hazardous to health in accordance with the *Globally Harmonised System of Classification and Labelling of Chemicals (GHS)* as adopted for industrial chemicals in Australia, workplace practices and control procedures consistent with provisions of State and Territory hazardous substances legislation should be in operation.

Emergency procedures

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

Disposal

- Where reuse or recycling are not appropriate, dispose of the notified chemical in an environmentally sound manner in accordance with relevant Commonwealth, state, territory and local government legislation.

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 final use concentration of the notified chemical exceeds 0.1% in household cleaning products;

or

(2) Under Section 64(2) of the Act; if
- the function or use of the chemical has changed from a fragrance ingredient in household cleaning products, or is likely to change significantly;
- the amount of chemical being introduced has increased, 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.

Safety Data Sheet
The SDSs of the notified chemical, and products containing the notified chemical, provided by the notifier were reviewed by NICNAS. The accuracy of the information on the SDSs remains the responsibility of the applicant.

ASSESSMENT DETAILS

1. APPLICANT AND NOTIFICATION DETAILS

APPLICANT(S)
Henkel Australia Pty Ltd (ABN: 82 001 302 996)
135-141 Canterbury Road
KILSYTH VIC 3137

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 exempt from publication.

VARIATION OF DATA REQUIREMENTS (SECTION 24 OF THE ACT)
Schedule data requirements are not varied.

PREVIOUS NOTIFICATION IN AUSTRALIA BY APPLICANT(S)
None

NOTIFICATION IN OTHER COUNTRIES
USA (2009)
Korea (2011)
China (2017)

2. IDENTITY OF CHEMICAL

MARKETING NAME(S)
Phenylethyl silicic acid ester

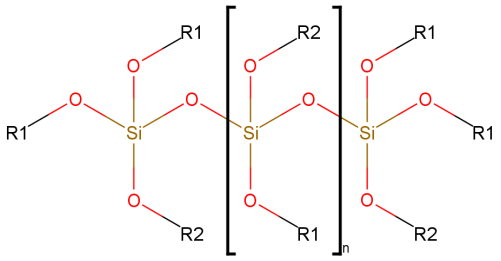
CAS NUMBER
891196-28-4

CHEMICAL NAME
Silicic acid, ethyl 2-phenylethyl ester

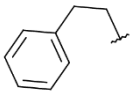
OTHER NAME(S)
Phenylethyl-KSE
Phenylethyl-Kieselsäureester
SAT 990180
SAT 980609
Polytetraphenylethoxysilan

MOLECULAR FORMULA
$C_8H_{10}O.xC_2H_6O.x$Unspecified

STRUCTURAL FORMULA



R2 

R1 

MOLECULAR WEIGHT

Number Average Molecular Weight (Mn)	844 g/mol
Weight Average Molecular Weight (Mw)	1,229 g/mol
Polydispersity Index (Mw/Mn)	1.5
% of Low MW Species < 1,000 g/mol	42.8
% of Low MW Species < 500 g/mol	9.5

ANALYTICAL DATA
Reference NMR, IR, GPC, UV spectra were provided.

3. COMPOSITION

DEGREE OF PURITY
> 96%

HAZARDOUS IMPURITIES/RESIDUAL MONOMERS

Chemical Name	Benzeneethanol		
CAS No.	60-12-8	*Weight %*	3-4
Hazardous Properties	Not listed on HCIS. ECHA (introducers classification): H302: Harmful if swallowed H312: Harmful in contact with skin H319: Causes serious eye irritation		

NON HAZARDOUS IMPURITIES/RESIDUAL MONOMERS (> 1% BY WEIGHT)
None

ADDITIVES/ADJUVANTS
None

4. PHYSICAL AND CHEMICAL PROPERTIES

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

Property	***Value***	***Data Source/Justification***
Melting Point	< -90 °C	Measured

Property	*Value*	*Data Source/Justification*
Boiling Point	350 °C at 101.3 kPa	Measured. Boiling and/or thermal decomposition occurred.
Density	1,139 kg/m^3 at 20 °C	Measured
Vapour Pressure	≤ 3.4 × 10^{-5} kPa at 20 °C	Estimated
Water Solubility	< 2 × 10^{-4} g/L at 20 °C	Measured (analogue LTD/2119)
Hydrolysis as a Function of pH	Not determined	Expected to hydrolyse in the environmental pH of 4-9
Partition Coefficient (n-octanol/water)	log Pow = > 5	Estimated using QSAR (US EPA, 2012). Due to unlimited 1-octanol solubility, partition coefficient could not be calculated
Adsorption/Desorption	Not determined	Due to poor solubility in water, the test could not be conducted
Dissociation Constant	Not determined	No dissociable functionality
Flash Point	123.5 °C at 101.3 kPa	Measured
Flammability	Not flammable	Measured
Autoignition Temperature	465 °C	Measured
Explosive Properties	Not determined	Contain no functional groups that would imply explosive properties
Oxidising Properties	Not determined	Contain no functional groups that would imply oxidative properties
Pyrophoric properties	Not pyrophoric	Measured

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

Reactivity
The notified chemical is designed to hydrolyse to silicic acid and the fragrance alcohol component during its use in household cleaning products.

Physical Hazard Classification
Based on the submitted physico-chemical data depicted in the above table, the notified chemical is not recommended for hazard classification according to the *Globally Harmonised System of Classification and Labelling of Chemicals (GHS),* as adopted for industrial chemicals in Australia.

The notified chemical has a flash point of 123.5 °C which is greater than 93 °C. Based on *Australian Standard AS1940* definitions for combustible liquid, the notified chemical may be considered as a Class C2 combustible liquid if the chemical has a flash point below the boiling point.

5. INTRODUCTION AND USE INFORMATION

MODE OF INTRODUCTION OF NOTIFIED CHEMICAL (100%) OVER NEXT 5 YEARS
The notified chemical will not be manufactured in Australia. The notified chemical will be imported as a component of fragrance oils at ≤ 12% concentration for local reformulation into household cleaning products, or as a component of finished household cleaning products at ≤ 0.1% 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 and Brisbane

IDENTITY OF RECIPIENTS
Pax Australia Pty Ltd
Jalco Household & Fabric Care

TRANSPORTATION AND PACKAGING

The notified chemical will be imported as a component of finished household cleaning products at ≤ 0.1% concentration packed in containers suitable for retail sale or as fragrance oil at ≤ 12% concentration in 200 L drums and 1,000 L intermediate bulk containers (IBCs). Finished consumer products containing the notified chemical will be transported primarily by road to retail stores in packages suitable for retail sale. Within Australia the drums and IBCs will be transported by road to industrial customers for reformulation.

USE

The notified chemical will be used as a fragrance ingredient in household cleaning products (such as detergents, fabric softeners and hard surface cleaners) at ≤ 0.1% concentration.

OPERATION DESCRIPTION

Reformulation

Reformulation of the fragrance oil containing the notified chemical at ≤ 12% concentration into finished consumer goods may vary depending on the type of product and may involve both automated and manual transfer steps. Typically, reformulation processes may incorporate blending operations that are highly automated and occur in a fully enclosed/contained environment, followed by automated filling of the reformulated end use products into containers of various sizes.

End use

End use products containing the notified chemical at ≤ 0.1% concentration will be used by consumers and professional cleaners. Depending on the nature of the product, these could be applied in 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

CATEGORY OF WORKERS

Category of Worker	*Exposure Duration (hours/day)*	*Exposure Frequency (days/year)*
Transport and storage	None	Incidental
Mixer	4	2
Drum handling	4	2
Drum cleaning/washing	4	2
Maintenance	4	1
Quality control	1	2
Packaging	4	2

EXPOSURE DETAILS

Transport and storage

Transport, storage and warehouse workers may come into contact with the notified chemical at ≤ 12% concentration in fragrance oils, or at ≤ 0.1% concentration in finished consumer products, only in the unlikely event of accidental rupture of containers.

Reformulation

During reformulation dermal, ocular and perhaps inhalation exposure of workers to the notified chemical at ≤ 12% concentration may occur during weighing and transfer stages, blending, quality control analysis and cleaning and maintenance of equipment. It is expected that exposure will be minimised through the use of mechanical ventilation and/or enclosed systems, and workers wearing personal protective equipment (PPE) such as protective clothing, eye protection, impervious gloves and respiratory protection, if inhalation exposure may occur.

End use

Exposure to the notified chemical in end use products at ≤ 0.1% concentration may occur in professions where the services provided involve the use of household cleaning products in the cleaning industry. The principal route of exposure will be dermal, while ocular and inhalation exposure are also possible. Professional cleaners may use

some PPE to minimise repeated exposure, and good hygiene practices are expected to be in place. If PPE is used, exposure of such workers is expected to be of a similar or lesser extent than that experienced by consumers using the products containing the notified chemical.

6.1.2. Public Exposure

There will be repeated exposure of the public to the notified chemical at ≤ 0.1% concentration through the use of household cleaning products. The main route of exposure will be dermal, while ocular and inhalation exposure are also possible, particularly if products are applied by spray.

6.2. Human Health Effects Assessment

The results from toxicological investigations conducted on the notified chemical are summarised in the following table. For details of the studies, refer to Appendix B.

Endpoint	*Result and Assessment Conclusion*
Acute oral toxicity – rat (OECD TG 420)	LD50 > 2,000 mg/kg bw; low toxicity
Skin irritation – rabbit (OECD TG 404)	non-irritating
Eye irritation – *in vitro* HET-CAM* (non OECD TG)	slightly irritating
Skin sensitisation – guinea pig, OET# (non OECD TG)	no evidence of sensitisation
Mutagenicity – bacterial reverse mutation (OECD TG 471)	non mutagenic

* HET-CAM: Hen's Egg Test – Chorioallantoic Membrane
# OET: Open epicutaneous test

Toxicokinetics
Dermal absorption of the notified chemical is expected to be limited based on the estimated low water solubility (< 0.2 mg/L) and high partition coefficient (log Pow of > 5).

Acute Toxicity
Based on a study conducted in rats, the notified chemical is of low acute oral toxicity.

Irritation and Sensitisation
In a skin irritation study conducted in rabbits, the notified chemical was found to be non-irritating.

In an *in vitro* eye irritation test (HET-CAM), the notified chemical was considered to be slightly-irritating based on an in-house irritation classification scheme.

In a guinea pig open epicutaneous test, no evidence of sensitisation to the notified chemical was observed at induction and challenge concentrations up to 100%.

Mutagenicity
The notified chemical was not mutagenic in a bacterial reverse mutation assay.

Health Hazard Classification
As only limited toxicity data were provided, the notified chemical cannot be classified according to the *Globally Harmonised System of Classification and Labelling of Chemicals* (GHS), as adopted for industrial chemicals in Australia.

6.3. Human Health Risk Characterisation

Based on the limited toxicity data provided, the notified chemical is expected to be of low acute oral toxicity, non-irritating to skin, slightly irritating to eyes and non-sensitising. No repeated dose toxicity data of the notified chemical was provided; however, dermal absorption is expected to be limited to cause systemic toxicity.

6.3.1. Occupational Health and Safety

Reformulation
Workers may experience dermal, ocular and perhaps inhalation exposure to the notified chemical at ≤ 12% concentration during reformulation. The use of local ventilation, enclosed/automated processes and PPE by workers (i.e., protective clothing, goggles, impervious gloves and respiratory protection, if inhalation exposure may occur) are expected to minimise the potential for exposure.

Therefore, under the occupational settings described, the risk to workers from use of the notified chemical is not considered to be unreasonable.

End use
Workers involved in professions where the services provided involve the use of household cleaning products in the cleaning industry may be exposed to the notified chemical at ≤ 0.1% concentration. Professional cleaners may use some PPE to minimise repeated exposure, and good hygiene practices are expected to be in place. The risk to such workers is expected to be of a similar or lesser extent than that experienced by consumers using various products containing the notified chemical. For details of the public health risk assessment see section 6.3.2 below.

6.3.2. Public Health
Members of the public will experience widespread and frequent exposure to the notified chemical at ≤ 0.1% concentration through daily use of household cleaning products. The main route of exposure is expected to be dermal, while ocular and inhalation exposure are also possible, particularly if products are applied by spray. In addition, the public may be similarly exposed to the fragrance alcohol components that are designed to be released from hydrolysis of the notified chemical during use.

Given the low end use concentration, local and systemic toxicity effects are not expected from exposure to the notified chemical or the hydrolysis products. Therefore, the risk to the public associated with use of the notified chemical at ≤ 0.1% concentration in household cleaning products is not considered to be unreasonable.

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 into Australia as a component of fragrance oils for local reformulation into household cleaning products, or as a component of finished household cleaning products. In general, the reformulation processes are expected to involve automated blending operations in an enclosed environment, followed by packing of the finished products into end use containers. Wastewater from reformulation equipment cleaning containing the notified chemical are expected to be disposed of to sewers via on-site wastewater treatment in accordance with local government regulations. Release of the notified chemical in the event of accidental spills or leaks during reformulation, storage and transport is estimated as 0.2% of the import volume and expected to be collected for disposal, in accordance with local government regulations.

RELEASE OF CHEMICAL FROM USE
The notified chemical is expected to be rapidly hydrolysed and the degradants are expected to be released to sewers across Australia as a result of their use in household cleaning products.

RELEASE OF CHEMICAL FROM DISPOSAL
Residues of the notified chemical in empty import and end use containers are likely to either share the fate of the containers and be disposed of to landfill or be released to the sewer system when containers are rinsed before recycling through an approved waste management facility.

7.1.2. Environmental Fate
The notified chemical is expected to be rapidly hydrolysed to silicic acid and the fragrance component during its use in household cleaning products. The majority of the degradants are expected to be released into the sewer system and treated at sewage treatment plants (STPs) before potential release to surface waters nationwide. The fragrance component of the notified chemical is volatile and is expected to volatilise to air. The half-life of the notified chemical in air is calculated to be ~12 minutes based on reactions with hydroxyl radicals (US EPA, 2012; AOPWIN v1.92). Therefore, the notified chemical or its degradants are not expected to persist in the air compartment.

The notifier has indicated that the notified chemical is not readily biodegradable (31% after 28 days, analogue – LTD/2119), but no study reports were provided. Without these reports, it is unknown if the silicic acid component, which is inherently not biodegradable, was factored into determining the biodegradability of the notified chemical.

Any residual notified chemical will continue to hydrolyse in STPs, environmental waters and sediment, to the corresponding silicic acid and fragrance component and is not expected to bioaccumulate. Ultimately, the notified chemical will degrade biotically and abiotically to form water and oxides of carbon and silicon.

7.1.3. Predicted Environmental Concentration (PEC)

The use pattern will result in most of the notified chemical being washed into the sewer. The predicted environmental concentration (PEC) has not been calculated since the notified chemical is expected to be rapidly hydrolysed to silicic acid and fragrance component during use.

7.2. Environmental Effects Assessment

The result from ecotoxicological investigations conducted on the notified chemical is summarised in the table below. Details of this study can be found in Appendix C.

Endpoint	*Result*	*Assessment Conclusion*
Daphnia Toxicity	48 h EC50 > 100 mg WAF*/L	Not toxic to aquatic invertebrates

*WAF: Water Accommodated Fraction

Based on the above ecotoxicological endpoint for the notified chemical, it is not expected to be harmful to aquatic organisms. Therefore, the notified chemical is not formally classified under the Globally Harmonised System of *Classification and Labelling of Chemicals* (GHS) for acute or chronic toxicity (United Nations, 2009).

7.2.1. Predicted No-Effect Concentration

The Predicted No-Effect Concentration (PNEC) of the notified chemical was not calculated as the notified chemical was not found to be toxic to aquatic organisms.

7.3. Environmental Risk Assessment

The notified chemical is expected to be rapidly hydrolysed to silicic acid and the fragrance component. The notified chemical and hydrolysis products are not toxic to daphnia. Therefore, based on the low hazard and reported use pattern, the notified chemical is not considered to pose an unreasonable risk to the environment.

APPENDIX A: PHYSICAL AND CHEMICAL PROPERTIES

Freezing Point < -90 °C

Method	EC Council Regulation No 440/2008 A.1 Melting/Freezing Temperature
Remarks	Determined using Differential Scanning Calorimetry (DSC)
Test Facility	Henkel (2018a)

Boiling Point 350 °C at 101.3 kPa

Method	EC Council Regulation No 440/2008 A.2 Boiling Temperature
Remarks	Determined using Differential Scanning Calorimetry (DSC)
Test Facility	Henkel (2018b)

Density 1,139 kg/m^3 at 20 °C

Method	OECD TG 109 Density of Liquids and Solids
Remarks	Determined using an oscillating densitometer
Test Facility	Henkel (2018c)

Vapour Pressure $\leq 3.4 \times 10^{-5}$ kPa at 20 °C

Method	EC Council Regulation No 440/2008 A.4 Vapour Pressure
Remarks	Calculation is based on the lowest possible boiling temperature (Grain Watson estimation method).
Test Facility	Henkel (2018d)

Water Solubility $< 2 \times 10^{-4}$ g/L at 20 °C (analogue – LTD/2119)

Method	OECD TG 105 Water Solubility EC Council Regulation No 440/2008 A.6 Water Solubility
Remarks	Column Elution Method
Test Facility	Henkel (2019a)

Flash Point 123.5 °C at 101.3 kPa

Method	EC Council Regulation No 440/2008 A.9 Flash Point
Remarks	Pre-test to determine the flash point was conducted using a rapid tester. Flash point tester was used to determine the flash point according to test method (S)21N04005.04 (Setaflash Series 7, 8 and 8 AC).
Test Facility	Henkel (2018e)

Flammability Not flammable

Method	EC Council Regulation No 440/2008 A.12 Flammability (Contact with Water)
Remarks	The test substance was exposed to either water or damp air and monitored for the release of gas.
Test Facility	Henkel (2019b)

Autoignition Temperature 465 °C

Method	EC Council Regulation No 440/2008 A.15 Auto-Ignition Temperature (Liquids and Gases)
Remarks	Small quantities of the test substance were squirted into a flask at various temperatures and autoignition of the vapour was monitored.
Test Facility	Henkel (2019c)

Pyrophoric properties of solids and liquids No pyrophoric properties

Method	EC Council Regulation No 440/2008 A.13 Pyrophoric properties of solids and liquids.
Remarks	The test substance was added to diatomaceous earth and brought into contact with air at ambient temperature. As no ignition was noted the test substance was added to filter paper and then exposed to air at ambient temperature.
Test Facility	Henkel (2019d)

APPENDIX B: TOXICOLOGICAL INVESTIGATIONS

B.1. Acute Oral Toxicity – Rat

TEST SUBSTANCE	Notified chemical
METHOD	OECD TG 420 Acute Oral Toxicity – Fixed Dose Procedure - 1992 EC Council Regulation No 440/2008 B.1 Acute Toxicity (Oral) - 1992
Species/Strain	Rat/Wistar SPF
Vehicle	Sesame oil
Remarks – Method	A separate sighting study and main study were performed for the notified chemical. In the sighting study, one female was dosed with 2,000 mg/kg bw of the notified chemical. Slight signs of toxicity were observed (pinched abdomen and piloerection) in the treated animal up to 24 hours after administration. Based on the results from the sighting study, a dose of 2,000 mg/kg bw was chosen for the main study. No major deviations from the test guideline were reported in either study. The testing laboratory was GLP compliant.

RESULTS

Group	*Number and Sex of Animals*	*Dose (mg/kg bw)*	*Mortality*
1	10 (5F/5M)	2,000	0/10

LD50	2,000 mg/kg bw
Signs of Toxicity	Pinched abdomen and piloerection were observed one hour after administration in all treated animals. Six hours after administration only piloerection was observed in all treated animals. All animals appeared normal from the Day 1 observation.
Effects in Organs	No abnormities were observed at necropsy
Remarks – Results	All animals showed expected body weight gain during the observation period.
CONCLUSION	The notified chemical is of low acute toxicity via the oral route.
TEST FACILITY	Scantox (1998)

B.2. Skin Irritation – Rabbit

TEST SUBSTANCE	Notified chemical
METHOD	OECD TG 404 Acute Dermal Irritation/Corrosion - 1992 EC Directive 2004/73/EC B.4 Acute Toxicity (Skin Irritation) - 1992
Species/Strain	Rabbit/New Zealand White
Number of Animals	3
Vehicle	None
Observation Period	72 hours
Type of Dressing	Semi-occlusive
Remarks – Method	No major deviations from the test guideline were reported. The test substance was used as supplied.
RESULTS	
Remarks – Results	No effects were observed on the treated skin of any animal.
CONCLUSION	The notified chemical is non-irritating to the skin.
TEST FACILITY	RCC (1999a)

B.3. Eye Irritation – *In Vitro* HET-CAM Test

TEST SUBSTANCE: Notified chemical

METHOD: The Hen's Egg Test on the Chorioallantoic Membrane (HET-CAM) Reaction-Time Method – Prior to OECD TG

Vehicle: None

Remarks – Method: The notified chemical was tested undiluted. The reference substance was 5% Texapon ASV (sodium magnesium lauryl-myristyl-6-ethoxy-sulfate).

The reaction-time method for HET-CAM was used to test the notified chemical. Approximately 300 µL of the notified chemical was added to six eggs with well-developed blood vessels. The notified chemical covered approximately 25% of the chorioallantoic membrane (CAM). The reaction-time period and reaction intensity of effects on the CAM like haemorrhage, lysis of the vessels and protein coagulation (intravascular and/or extravascular) were visually evaluated.

An internal classification scheme for irritating properties was used by the study authors to classify the notified chemical as described below:

Relative Irritation Potential	*Evaluation*
≤ 0.8	slightly irritating
> 0.8 - < 1.2	moderately irritating
≥ 1.2 - < 2.0	irritating
≥ 2	severely irritating

The testing laboratory was GLP compliant.

RESULTS

Test material	*Relative Irritation Potential*	*Evaluation**
Test substance	0.00	slightly irritating
Reference Item	1.00 (± 0.06)	moderately irritating

*Based on internal classification scheme for irritating properties

Remarks – Results: No individual scores were provided.

The study authors considered the notified chemical to be slightly irritating.

CONCLUSION: The notified chemical was considered slightly irritating under the conditions of the test.

TEST FACILITY: Henkel (2007)

B.4. Skin Sensitisation – Guinea Pig, OET

TEST SUBSTANCE: Notified chemical

METHOD: OECD TG 406 Skin Sensitisation – Open Epicutaneous Test (OET) – non OECD TG

Species/Strain: Guinea pig/Himalayan spotted

PRELIMINARY STUDY: Maximum non-irritating concentration:
Topical: 100%

MAIN STUDY

Number of Animals: Test Group: 6F Control Group: 6F

Vehicle: PEG 400

Positive Control: Not conducted in parallel with the notified chemical. The positive control was 2-mercaptobenzothiazole.

INDUCTION PHASE	Induction concentration: Topical: 3%, 10%, 30% and 100%
Signs of Irritation	Discrete/patchy erythema was observed in animals after repeated application of the notified chemical at concentrations of 100% and 30% during the induction phase.
CHALLENGE PHASE	
1st Challenge	Topical: 3%, 10%, 30% and 100%
2nd Challenge	Topical: 3%, 10%, 30% and 100%
Remarks – Method	The test substance (0.1 mL) was applied to the shaved right flanks of guinea pigs (skin area 7 cm^2) for 8 weeks. The applications were repeated daily, 5 times during the first week, once during the second week, 5 times per week during weeks 5, 6 and 7 and twice during week 8, using the same skin site. Groups of six test animals each, were treated with only one test substance concentration. After induction on Day 71, the animals were challenged at four concentrations on the shaved left flank using 0.025 mL of test substance to a skin area of 2 cm^2. The reactions were read at 24, 48 and 72 hours. Control animals were treated with the vehicle (PEG 400) only.
RESULTS	
Remarks – Results	No skin reactions were observed in animals induced with the notified chemical at up to 100% concentration, and at challenge concentrations up to 100%. Body weight changes of all test animals were within the normal range.
CONCLUSION	There was no evidence of reactions indicative of skin sensitisation to the notified chemical under the conditions of the test.
TEST FACILITY	RCC (1999b)

B.5. Genotoxicity – Bacteria

TEST SUBSTANCE	Notified chemical
METHOD	OECD TG 471 Bacterial Reverse Mutation Test - 1983 Plate incorporation procedure
Species/Strain	*Salmonella typhimurium*: TA1538, TA1535, TA1537, TA100 and TA98
Metabolic Activation System	S9 mix from phenobarbitone/β-naphthoflavone induced rat liver
Concentration Range in Main Test	a) With metabolic activation: 8-5,000 µg/plate b) Without metabolic activation: 8-5,000 µg/plate
Vehicle	Dimethyl sulfoxide (DMSO)
Remarks – Method	No major deviations from the test guideline were reported. Positive controls: With metabolic activation: 2-aminoanthracene (TA98, TA100, TA1535, TA1537 and TA1538) Without metabolic activation: sodium azide (TA100 and TA1535), 9-aminoacridine (TA1537), 4-nitro-o-phenylenediamine (TA98 and TA1538).

RESULTS

Metabolic Activation	*Test Substance Concentration (µg/plate) Resulting in:*			
	Cytotoxicity in Preliminary Test	*Cytotoxicity in Main Test*	*Precipitation*	*Genotoxic Effect*
Absent				
Test 1	> 5,000	–	> 5,000	Negative

Test 2	–	> 5,000	> 5,000	Negative
Present				
Test 1	> 5,000	–	> 5,000	Negative
Test 2	–	> 5,000	> 5,000	Negative

Remarks – Results

No significant increases in the frequency of revertant colonies were observed for any of the bacterial strains, with any dose of the test substance, either with or without metabolic activation.

The positive and negative controls provided a satisfactory response confirming the validity of the test system.

CONCLUSION

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

TEST FACILITY

Henkel (1998)

APPENDIX C: ENVIRONMENTAL FATE AND ECOTOXICOLOGICAL INVESTIGATIONS

C.1. Ecotoxicological Investigations

C.1.1. Acute Toxicity to Aquatic Invertebrates

TEST SUBSTANCE	Notified chemical
METHOD	OECD TG 202 Daphnia sp. Acute Immobilisation Test and Reproduction Test – Static
Species	*Daphnia magna*
Exposure Period	48 hours
Auxiliary Solvent	None
Water Hardness	Not reported
Analytical Monitoring	HPLC
Remarks – Method	The study was carried out in accordance with the test guidelines and GLP. Due to the low water solubility of the notified chemical, water-accommodated fractions (WAF) were prepared. A nominal load (100 mg) of the test substance was added to dilution water and stirred for 24 hours. After this period the aqueous phase was transferred by a pipette and used for the test. The test was performed as a limit-test with the concentrations 100 and 10 mg/L. A positive control (potassium dichromate) was run.

RESULTS

Concentration (mg WAF/L)		*Number of D. magna*	*Number Immobilised*	
Nominal	*Actual*		*24 h*	*48 h*
10	0.5	20	0	0
100	0.5	20	0	0

LC50	> 100 mg WAF/L at 48 hours
NOEC (or LOEC)	100 mg/L at 48 hours
Remarks – Results	The validity criteria of the test were met. The dissolved O_2 was maintained above 9.0 mg/L throughout the test. The pH was maintained at 8.1. The temperature was maintained at 20 °C. The results from the positive control with potassium dichromate were within the normal range for the reference item (1.9 mg/L). Hydrolysis of the notified chemical during preparation and testing was not taken into account and therefore the toxicity is related to the notified chemical and its degradants.
CONCLUSION	The notified chemical is not toxic to aquatic invertebrates up to its water solubility limit.
TEST FACILITY	Henkel (2000)

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