File No: LTD/1674

July 2013

NATIONAL INDUSTRIAL CHEMICALS NOTIFICATION AND ASSESSMENT SCHEME (NICNAS)

PUBLIC REPORT

Fatty acids, coco, reaction products with N1-N1-dimethyl-1,3-propanediamine and 3-(2-oxiranylmethoxy)propyl group-terminated [(phenylsilylidyne)tris(oxy)tris[di-Me siloxanes], lactates (salts) (INCI name: Silicone Quaternium-22)

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

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

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

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Director
NICNAS

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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/1674	Brenntag Australia Pty Ltd	Fatty acids, coco, reaction products with N1-N1-dimethyl-1,3-propanediamine and 3-(2-oxiranylmethoxy)propyl group-terminated [(phenylsilylidyne)tris(oxy)tris[di-Me siloxanes], lactates (salts) (INCI name: Silicone Quaterium-22))	ND*	≤ 1 tonne per annum	Component of hair care products

*ND = not determined

CONCLUSIONS AND REGULATORY OBLIGATIONS

Hazard classification

Based on the available information, the notified polymer is not recommended for classification according to the *Globally Harmonised System for the Classification and Labelling of Chemicals* (GHS), as adopted for industrial chemicals in Australia, or the *Approved Criteria for Classifying Hazardous Substances* (NOHSC, 2004).

Human health risk assessment

Under the conditions of the occupational settings described, the notified polymer is not considered to pose an unreasonable risk to the health of workers.

When used at < 1% in hair care products, the notified polymer is not considered to pose an unreasonable risk to public health.

Environmental risk assessment

On the basis of the PEC/PNEC ratio and assessed use pattern, the notified polymer is not expected 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 safe work practices to minimise occupational exposure during handling of the notified polymer during reformulation processes:
  - Avoid contact with skin and eyes

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

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

- If products and mixtures containing the notified polymer are classified as hazardous to health in accordance with the *Globally Harmonised System for the 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.

Disposal

- The notified polymer should be disposed of to landfill.

Emergency procedures

- Spills or accidental release of the notified polymer 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 polymer 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 polymer has a number-average molecular weight of less than 1000;
  - the method of manufacture of the notified polymer changes, such that a significant proportion of low molecular weight species (< 1000 Da) will be present;

or

(2) Under Section 64(2) of the Act; if
  - the function or use of the polymer has changed from a component of hair care products or is likely to change significantly;
  - the amount of polymer being introduced has increased from 1 tonne per annum, or is likely to increase, significantly;
  - the polymer has begun to be manufactured in Australia;
  - additional information has become available to the person as to an adverse effect of the polymer 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 (M)SDS of the notified polymer provided by the notifier was reviewed by NICNAS. The accuracy of the information on the (M)SDS remains the responsibility of the applicant.

ASSESSMENT DETAILS

1. APPLICANT AND NOTIFICATION DETAILS

APPLICANT(S)
Brenntag Australia Pty Ltd (ABN: 84 117 996 595)
262 Highett Road
HIGHETT ROAD VIC 3190

NOTIFICATION CATEGORY
Limited: Synthetic polymer with Mn ≥ 1000 Da.

EXEMPT INFORMATION (SECTION 75 OF THE ACT)
Data items and details claimed exempt from publication: other names, molecular weight, analytical data, degree of purity, polymer constituents, residual monomers and identity of recipient.

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)
No

Notification in Other Countries
Canada (2012)

2. IDENTITY OF CHEMICAL

Marketing Name(s)
Abil T Quat 60 (contains 65% notified polymer)

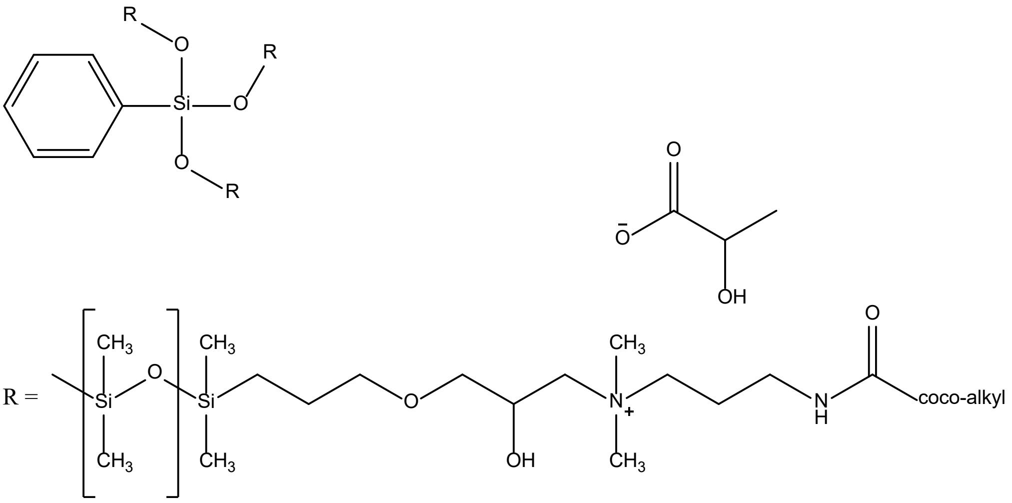
CAS Number
946846-36-2

Chemical Name
Fatty acids, coco, reaction products with N1-N1-dimethyl-1,3-propanediamine and 3-(2-oxiranylmethoxy)propyl group-terminated [(phenylsilylidine)tris(oxy)tris[di-Me siloxanes], lactates (salts)

Other Name(s)
Silicone Quaternium-22 (INCI name)
Triquaternary polydimethyl siloxane

Molecular Formula
Unspecified

Structural Formula



Molecular Weight
> 1,000 Da

Analytical Data
Reference GPC, NMR and IR spectra were provided.

3. COMPOSITION

Degree of Purity > 90%

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: Clear, yellowish highly viscous fluid

Property	Value	Data Source/Justification
Melting Point/Freezing Point	< -80 °C	Measured
Boiling Point	Decomposition without boiling from ~ 175 °C at 101.3 kPa	Measured
Density	997 kg/m^3 at 20 °C	Measured
Vapour Pressure	< 1.5 x 10^{-3} Pa at 20 °C	Measured
Water Solubility	< 1.0 x 10^{-3} g/L at 20 °C	Measured. Expected to be low based on its predominantly hydrophobic nature.
Hydrolysis as a Function of pH	Not determined	The notified polymer does not contain readily hydrolysable functionalities and is not expected to hydrolyse under environmental conditions (pH 4-9)
Partition Coefficient (n-ocatanol/water)	Estimated	log Pow > 6.0 at 20 °C
Adsorption/Desorption	log K_{oc} > 5	Calculated
Dissociation Constant	Not determined	The notified polymer is a salt and is ionised in this form
Flash Point	150 °C at 1013 hPa (closed cup)	Measured
Flammability	Not determined	Not expected to be flammable based on flash point
Autoignition Temperature	405 °C	Measured
Explosive Properties	Not determined	Contains no functional groups that would imply explosive properties
Oxidising Properties	Not determined	Contains no functional groups that would imply oxidising properties

DISCUSSION OF PROPERTIES

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

Reactivity

The notified polymer is expected to be stable under normal conditions of use.

Physical hazard classification

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

5. INTRODUCTION AND USE INFORMATION

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

The notified polymer will be imported into Australia as a component of the product Abil T Quat 60, containing the notified polymer at 65% 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 or Melbourne

IDENTITY OF MANUFACTURER/RECIPIENTS

Brenntag Australia Pty Ltd

TRANSPORTATION AND PACKAGING

Abil T Quat 60 (containing 65% notified polymer), will be transported from the port to reformulator warehouses by road in 50 kg pails or 200 kg drums. Reformulated end use products (containing < 1% notified polymer) will be transported by road in 125 mL plastic bottles inside cardboard boxes to distribution warehouses for sale to retailers.

USE

The notified polymer will be used as a conditioning agent in hair care products such as shampoo and conditioner at < 1% concentration. The products are expected to be used by the public and professionals (such as hairdressers).

OPERATION DESCRIPTION

Reformulation

Abil T Quat 60 (containing 65% notified polymer), will be reformulated into various end use hair care products containing < 1% notified polymer. The process will vary depending on the nature of the product and may involve both automated and manual transfer steps. A typical formulation process will likely involve manual weighing of the notified polymer into a closed system mixing tank and then automated packaging of the formulated products into plastic containers for retail sale.

End use

The finished hair care products (containing < 1% notified polymer) will be distributed to retail outlets for sale to the public and professionals such as hair dressers. Application of products will be by hand.

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)*
Manufacturing operator	1	20
Laboratory analyst	1	6
Hairdresser / store persons	Unspecified	Unspecified

EXPOSURE DETAILS

Transport and storage

Transport and storage workers are not likely to be exposed to the imported product containing the notified polymer (at 65% concentration) except in the event of accidental rupture of containers.

Formulation of hair care products

During formulation of hair care products, dermal and ocular exposure of workers to the notified polymer (at 65% concentration) may occur during weighing and transfer stages, blending, quality control analysis and cleaning and maintenance of equipment. Exposure is expected to be minimised through the use of mechanical ventilation and/or enclosed systems and through the use of personal protective equipment (PPE) such as coveralls, safety glasses and impervious gloves.

Inhalation exposure is unlikely as the notified ingredient is supplied as a liquid and the finished product is a liquid containing the notified chemical (imported at 65%).

End-use

Hairdressers and hair salon workers may experience dermal and accidental ocular exposure to the notified polymer at < 1% concentration during application of hair care products to the hair of customers. Such professionals 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 hair care products containing the notified polymer.

6.1.2. Public Exposure

There will be widespread and repeated exposure of the public to the notified polymer (at < 1% concentration) through the use of the hair care products (shampoos and conditioners). The principal route of exposure will be dermal.

6.2. Human Health Effects Assessment

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

Endpoint	*Result and Assessment Conclusion*
Rat, acute oral toxicity	LD50 > 2000 mg/kg bw; low toxicity
Rabbit, skin irritation	slightly irritating
Eye irritation (in vitro)	slightly irritating
Guinea pig, skin sensitisation – adjuvant test	no evidence of sensitisation
Mutagenicity – bacterial reverse mutation	non mutagenic

Toxicokinetics, metabolism and distribution.

The notified polymer is a high molecular weight salt (> 1000 Da) with a low proportion of low molecular weight species (< 3% with molecular weight < 1000 Da) and limited water solubility (< 1 mg/L). These characteristics are expected to limit absorption across biological membranes. Given the low vapour pressure of the notified polymer, inhalation exposure would only be expected if aerosols are formed. If inhalation exposure were to occur the notified polymer would be expected to be cleared from the lungs.

Acute toxicity.

The notified polymer was found to be of low acute oral toxicity in rats. No mortalities or adverse effects were observed. The treated animals displayed expected weight gains during the study.

Irritation and sensitisation.

The notified polymer was found to be slightly irritating to the skin of rabbits.

The notified polymer was predicted to be slightly irritating to the eye in a HET-CAM test. The HET-CAM assay has not yet been validated as a replacement test for the *in vivo* Draize test, and is not to be used for regulatory hazard classification purposes, based on a lack of adequate data (ICCVAM, 2009).

There was no evidence of reactions indicative of skin sensitisation to the notified polymer in a guinea pig maximisation study.

Mutagenicity/Genotoxicity.

No toxicologically significant increases in the frequency of revertant colonies were recorded for any of the bacterial strains, with any dose of the test material, either with or without metabolic activation, in a reverse mutation study.

Repeat dose toxicity

No repeat dose toxicity data was provided for the notified polymer. The notified polymer is not expected to be significantly dermally absorbed due to its high molecular weight, low proportion of low molecular weight species and low water solubility. As such, systemic toxicity following dermal exposure to the notified polymer is expected to be low.

Health hazard classification

Based on the available information, the notified polymer is not recommended for classification according to the *Globally Harmonised System for the Classification and Labelling of Chemicals (GHS),* as adopted for industrial chemicals in Australia, or the *Approved Criteria for Classifying Hazardous Substances* (NOHSC, 2004).

6.3. Human Health Risk Characterisation

6.3.1. Occupational Health and Safety

The notified polymer is slightly irritating to the skin and eyes. Exposure via inhalation is not expected given the low estimated vapour pressure of the notified polymer. Based on the high molecular weight of the notified polymer, the possibility of dermal absorption following exposure is limited.

Reformulation
Compounders and laboratory staff involved in the formulation of cosmetic products may come in contact with the notified polymer at 65% concentration. Exposure is expected to be limited during product formulation by the engineering controls, the use of PPE, and the use of enclosed and automated processes. Given the low hazardous nature of the notified polymer and the control measures in place to limit exposure, the notified polymer is not considered to pose an unreasonable risk to reformulation workers.

End-use
Hairdressers and salon workers will handle the notified polymer at < 1% concentration in hair care products, similar to public use. Therefore, the risk for these professionals who regularly use products containing the notified polymer is expected to be of a similar or lesser extent than that experienced by members of the public who use such products on a regular basis. For details of the public health risk assessment, see Section 6.3.2.

Based on the information available, the risk to workers associated with use of the notified polymer at < 1% concentration in hair care products is not considered to be unreasonable.

6.3.2. Public Health

The general public will be repeatedly exposed to the notified polymer during the use of hair care products containing the notified polymer at < 1% concentration. The principal route of exposure will be dermal.

Local effects
Based on the information available, the notified polymer is slightly irritating to the skin and eyes. However, at the proposed use concentration of < 1% in hair care products, irritation effects are not expected.

Systemic effects
There are no repeat dose toxicity data available for the notified polymer. However, given the high molecular weight of the notified polymer dermal absorption is not expected.

Therefore, based on the information available, the risk to the public associated with the use of the notified polymer at < 1% concentration in hair care 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 polymer is expected to be imported into Australia as a component of a formulation for hair care products. The release of the notified polymer from local reformulation or repackaging (< 5% of the total annual volume) is likely to be treated in an on-site treatment plant. The sludge and liquid effluent discharged from the on-site treatment plant is anticipated to be disposed of to landfill and trade waste, respectively.

RELEASE OF CHEMICAL FROM USE
The notified polymer is a component of hair care products, which will be directly applied to the consumer's hair. The hair shampoo/conditioner is likely to be rinsed off and enter the drainage/sewerage system, where it will be directed to various waste water treatment facilities

RELEASE OF CHEMICAL FROM DISPOSAL
The hair conditioner bottles, containing the notified polymer, are expected to be sent for recycling wherever possible once the bottle is no longer to be used. However, as end users are the general public, a proportion of containers are anticipated to be sent to landfill. It is expected that there may be residual notified polymer of up to 0.5% (the total annual volume) remaining within the bottles.

7.1.2. Environmental Fate

No environmental fate data were submitted. The notified polymer is not considered readily biodegradable based on its molecular structure and molecular weight. It is anticipated that almost all of the imported product containing the notified polymer will go to the sewage system via rinsing after hair application. Since the notified polymer has a tendency to sorb to sediment/sludge based on its log Pow value and cationicity, it is likely to mainly partition to sludge and be disposed of to landfill. Therefore, most of the notified polymer is expected to be removed from the influent and it is not likely to be significantly bioavailable to aquatic organisms. Given that the notified polymer has a high molecular weight, it is not expected to bioaccumulate as it is too large to cross the biological membranes. It was assumed that 90% of the notified polymer partitions to sludge in sewage treatment plants (STPs) as it is a polymer with cationicity (Boethling and Nabholz, 1997). Based on this, it is expected that no significant amount of the imported notified polymer will be end up in the surface waters.

7.1.3. Predicted Environmental Concentration (PEC)

The calculation for the Predicted Environmental Concentration (PEC) is summarised in the table below. Based on the reported use in hair care products, it is assumed as a worst case scenario that 100 % of the total import volume of polymer would be released to sewer on a nationwide basis over 365 days per year. It was assumed that 0% of the notified polymer partitions to sludge in STPs for this scenario, although it is a cationic polymer.

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)	22.613	million
Removal within STP	0%	
Daily effluent production:	4,523	ML
Dilution Factor - River	1.0	
Dilution Factor - Ocean	10.0	
PEC - River:	0.61	μg/L
PEC - Ocean:	0.06	μg/L

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 polymer 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 0.61 μg/L may potentially result in a soil concentration of approximately 4.04 μg/kg. Assuming accumulation of the notified polymer in soil for 5 and 10 years under repeated irrigation, the concentration of notified polymer in the applied soil in 5 and 10 years may be approximately 20.2 μg/kg and 40.4 μg/kg, respectively. However, these are expected to be maximum values as a significant proportion is expected to be disposed of to landfill as sludge.

7.2. Environmental Effects Assessment

No ecotoxicological data were submitted for the notified polymer. Cationic polymers are known to be toxic to aquatic life. Ecotoxicological endpoints for the notified polymer were calculated based on Structure Activity Relationships (SARs) equations assuming a worst case cationic charge density for the polymer (Boethling and Nabholz, 1997). The toxicity endpoints were predicted based on the tests conducted in standard aquatic toxicity testing media without any mitigation. The results are summarised in the table below.

Endpoint	*Results*	*Assessment conclusion*
Acute toxicity		
Fish	LC50 (96 h) = 14.4 mg/L	Predicted to be harmful to fish
Daphnia	LC50 (48 h) = 35.1 mg/L	Predicted to be harmful to aquatic invertebrates
Algae	EC50 (96 h) = 3.3 mg/L	Predicted to be toxic to algae
Chronic toxicity		
Fish	ChV = 0.8 mg/L*	Potentially toxic to fish with long lasting effects
Daphnia	ChV = 2.5 mg/L*	Not expected to be harmful to aquatic invertebrates
Algae	ChV = 0.9 mg/L*	Potentially toxic to algae with long lasting effects

* ChV = (LOEC × NOEC)½

The SARs estimation endpoints indicate that the notified polymer is potentially toxic to aquatic organisms. However, the actual toxicity of the notified polymer to aquatic life may be overestimated by SARs estimation used here as surface waters tend to have higher total organic content (TOC) and dissolved organic content (DOC) than what is used in standard aquatic toxicity testing media. The predicted acute toxicity values of all three test species for the notified polymer are higher than the solubility limit and the notified polymer may not soluble enough to have the predicted effect. However, the chronic toxicity values for fish and algae are less than the solubility limit and have been used unmitigated for the purpose of risk assessment. Classification should be based on actual toxicity endpoints and, therefore, the notified polymer has not been formally classified under the Globally Harmonised System of Classification and Labelling of Chemicals (GHS) (United Nations, 2009).

7.2.1. Predicted No-Effect Concentration

The predicted no-effect concentration (PNEC) has been calculated from the most conservative endpoint (fish, ChV) for the notified polymer and an assessment factor of 50. A conservative assessment factor is appropriate, in this case, as although chronic endpoints (ChV = (LOEC × NOEC)^{½}) for three trophic levels are available, these chronic endpoints are greater than no-observed effect concentrations (NOECs).

Predicted No-Effect Concentration (PNEC) for the Aquatic Compartment		
NOEC (Fish).	0.8	mg/L
Assessment Factor	50	
PNEC:	16	μg/L

7.3. Environmental Risk Assessment

Risk Assessment	PEC μg/L	PNEC μg/L	Q
Q - River:	0.61	1	0.038
Q - Ocean:	0.06	16	0.004

The Risk Quotients (Q = PEC/PNEC) for a worst case discharge scenario have been calculated to be < 1 for the river and ocean compartments. The notified polymer is not expected to be readily biodegradable or bioaccumulate in the environment. The notified polymer is not likely to significantly bioavailable as it is expected to be removed from the water column due to its strong potential to adsorb on suspended solids and sediments. The notified polymer is unlikely to result in ecotoxicologically significant concentrations in aquatic environment from the assessed use pattern. Therefore, it is expected that there is no unreasonable risk to the aquatic environment from the assessed use scenario.

APPENDIX A: PHYSICAL AND CHEMICAL PROPERTIES

Melting Point/Freezing Point < -80 °C

Method	OECD TG 102 Melting Point/Melting Range. EC Council Regulation No 440/2008 A.1 Melting/Freezing Temperature.
Remarks	The melting point of the test substance was determined using differential scanning calorimetry (DSC).
Test Facility	NOTOX B.V (2012)

Boiling Point Decomposes without boiling from ~175 °C at 101.3 kPa

Method	OECD TG 103 Boiling Point. EC Council Regulation No 440/2008 A.2 Boiling Temperature.
Remarks	The boiling temperature could not be determined as the test substance decomposed at temperatures > 175ºC.
Test Facility	NOTOX B.V (2012)

Density 997 kg/m^3 at 20 °C

Method	OECD TG 109 Density of Liquids and Solids. EC Council Regulation No 440/2008 A.3 Relative Density.
Remarks	The density of the test substance was determined using the gas comparison pycnometer method.
Test Facility	NOTOX B.V (2012)

Vapour Pressure $< 1.5 \times 10^{-3}$ Pa at 20 °C

Method	OECD TG 104 Vapour Pressure. EC Council Regulation No 440/2008 A.4 Vapour Pressure.
Remarks	The vapour pressure of the test substance was determined by the isothermal thermogravimetric effusion method.
Test Facility	NOTOX B.V (2012)

Water Solubility $< 1.0 \times 10^{-3}$ g/L at 20 °C

Method	OECD TG 105 Water Solubility
Remarks	Flask Method. After the stirring period, undissolved test substance was observed in the test sample.
Test Facility	NOTOX B.V (2012)

Partition Coefficient (n-octanol/water) log Pow > 6 at 20 °C

Method	OECD TG 107 Partition Coefficient (n-octanol/water)
Remarks	Estimation Method. Test substance was shaken with n-octanol at the nominal concentrations of 10.8 g/L, 105 g/L and 1042 g/L at 20.6 ±0.5 °C for 1 day and then, the test samples were usually interpreted. After the shaking period, no undissolved test substance was observed in the n-octanol test samples of 10.8 g/L and 105 g/L, as they were clear colourless solutions. However, the test sample of 1042 g/L appeared viscous slight yellow clear solution. It was concluded that the n-octanol solubility of the test substance was 1.0×10^3 g/L The Pow value was estimated from the quotient of the n-octanol and the water solubility of the test substance
Test Facility	NOTOX B.V (2012)

Adsorption/Desorption $\log K_{oc} = \log K_{oc} > 5$

Method	QSAR calculation method
Remarks	Based on the water solubility of the test substance ($< 1.0 \times 10^{-3}$ g/L at 20 °C), the test substance was classified as predominantly hydrophobic.

For this chemical class, the log Koc is given as:

log Koc = 0.81 log Pow + 0.1

The logarithm of the partition coefficient (log Pow) of the test substance is > 6.0. Using these values, the Koc of the test substance is > 9.1 × 104 and log Koc > 5.0.

Test Facility NOTOX B.V (2012)

Flash Point 150 °C at 1013 hPa

Method EC Council Regulation No 440/2008 A.9 Flash Point.

Remarks The flash point of the test substance was determined using a model APM-7 Pensky-Martens closed cup flash-point tester.

Test Facility NOTOX B.V (2012)

Autoignition Temperature 405 °C

Method EC Council Regulation No 440/2008 A.15 Auto-Ignition Temperature (Liquids and Gases).

Remarks The Autoignition of the test substance was determined using a commercially available autoignition temperature apparatus (Chilworth Technology).

Test Facility NOTOX B.V (2012)

APPENDIX B: TOXICOLOGICAL INVESTIGATIONS

B.1. Acute toxicity – oral

TEST SUBSTANCE	Notified Polymer
METHOD	OECD TG 423 Acute Oral Toxicity – Acute Toxic Class Method.
Species/Strain	Rat/White Wistar
Vehicle	Sesame oil
Remarks - Method	No significant protocol deviations.

RESULTS

Group	*Number and Sex of Animals*	*Dose mg/kg bw*	*Mortality*
I	6 females	300	0
II	6 females	2000	0

LD50	> 2000 mg/kg bw
Signs of Toxicity	None
Effects in Organs	None
Remarks - Results	No mortalities or adverse effects were observed following dosing with the test substance. The animals displayed expected body weight gains during the study.
CONCLUSION	The notified polymer is of low toxicity via the oral route.
TEST FACILITY	Stockhausen GmbH (2008a)

B.2. Irritation – skin

TEST SUBSTANCE	Notified Polymer
METHOD	OECD TG 404 Acute Dermal Irritation/Corrosion.
Species/Strain	Rabbit/New Zealand White
Number of Animals	2 females and 1 male
Vehicle	Test substance administered as supplied
Observation Period	7 days
Type of Dressing	Semi-occlusive.
Remarks - Method	Due to the male test animal dying during the acclimatization period, the test commenced with the two female test animals and completed two months later with an additional male test animal. Observations were made at 1, 24 and 48 hours and 7 days after removal of the test patch.

RESULTS

Lesion	*Mean Score* Animal No.*			*Maximum Value*	*Maximum Duration of Any Effect*	*Maximum Value at End of Observation Period*
	1	2	3			
Erythema/Eschar	0.33	1.67	1.67	2	< 7 days	0
Oedema	0	0.67	0	1	< 72 hrs	0

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

Remarks - Results	Well-defined erythema was observed for 2 animals up to the 48-hour observation period. Very slight erythema was still observed for these two animals at the 72-hour observation period. The remaining animal only showed very slight erythema up to the 24-observation period. In addition one animal showed very slight oedema formation. All symptoms of irritation had resolved at the 7-day observation period.

The test authors reported that there were no signs of systemic toxicity caused by the test substance. Body weights gain was positive and within normal ranges.

CONCLUSION The notified polymer is slightly irritating to the skin.

TEST FACILITY Stockhausen GmbH (2008b)

B.3. Irritation – eye

TEST SUBSTANCE Notified Polymer

METHOD The Hen's Egg Test – Utilizing the Chorioallantoic Membrane (HET-CAM) Test. Modification of that described by Luepke (1992).

Species/Strain SPAFAS chicken eggs

Remarks - Method Six eggs were fertilised and incubated for the test substance, negative and positive controls readings taken at 0.5, 2 and 5 mins. The eggs were incubated at 37.5 ± 0.5°C and a relative humidity of 62.5% (±7.5%) in an automatic, rotating incubator for 9 days. After 9 days, the shell over the air sac of each egg was removed, wetted with physiological saline at room temperature for approximately 1 minute and the CAM was removed with forceps. A 200 µL solution of the test substance (undiluted) was applied to each CAM and effects of vascular injection, haemorrhage and coagulation were observed over a period of 5 mins and scored according to the maximum scores shown in the following table.

	Scores at time (min):		
Effect	0.5	2	5
Vascular injection	5	3	1
Haemorrhage	7	5	3
Coagulation	9	7	5

Each reaction type can be recorded only once for each CAM, therefore the maximum score per CAM is 21. The mean score was determined for all CAMs similarly tested.

Scoring is according to severity and time needed for the effect to occur. The earlier a symptom is recorded the higher the numerical value is assigned to it. The order of the severity of the endpoints is as follows: Coagulation > Haemorrhage > Vascular Injection.

The duration of application with the test substance was not reported. The positive control used in the test was Texapon ASV 70 (sodium magnesium lauryl myristyl-6-ethoxy-sulfate) diluted to 5% with tap water. The negative control used in the test was tap water.

RESULTS

Test Solution	*Average Irritation score*
Tap water	0.0
Notified polymer	4.5
5% Texapon ASV (sodium magnesium lauryl-myristy1-6-ethoxy-sulfate)	9.3

Remarks - Results Vascular injection of the CAM 2 minutes following treatment was observed in all six eggs. Haemorrhage of the CAM 5 minutes following treatment with the notified polymer was observed in three eggs. This resulted in an irritation score of 4.5 out of a possible 21. In comparison, a score of 9.3 was reported for the positive control Texapon ASV at 5% concentration which is known to be slightly irritating *in vivo*. Therefore, a score of 4.5 for the notified polymer is predicted to

	be slightly irritating.
CONCLUSION	The notified polymer is slightly irritating to the eye.
TEST FACILITY	Stockhausen GmbH (2008c)

B.4. Skin sensitisation

TEST SUBSTANCE	
METHOD	OECD TG 406 Skin Sensitisation – Guinea Pig Maximisation Test
Species/Strain	Guinea pig/Hartley
PRELIMINARY STUDY	Maximum Non-irritating Concentration: intradermal: 0.5% (gave a slight reaction) topical: 1%
MAIN STUDY	
Number of Animals	Test Group: 10 females Control Group: 5 females
INDUCTION PHASE	Induction Concentration: intradermal: 0.5% topical: 100%
Signs of Irritation	Slight skin irritation was observed following both intradermal and topical induction.
CHALLENGE PHASE	
1st challenge	topical: 1%
2nd challenge	topical: 1%
Remarks - Method	Sesame oil was used as the vehicle.

RESULTS

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

Remarks - Results	No deaths occurred during the study. Apart from crust formation at the injection sites after intradermal injection, there were no substance-related signs of toxicity during the study. Body weight development of the test animals was reported to be positive and within normal ranges. Visible changes in the skin at treated sites were observed in two test animals during the challenge (discrete erythema and hardly detectable swelling), but these were temporary and were absent in the rechallenge, leading to the test authors conclusion that the responses were due to skin irritation rather than an immune response.
CONCLUSION	There was no evidence of reactions indicative of skin sensitisation to the notified polymer under the conditions of the test.
TEST FACILITY	Stockhausen GmbH (2008d)

B.5. Genotoxicity – bacteria

TEST SUBSTANCE	Notified Polymer
METHOD	OECD TG 471 Bacterial Reverse Mutation Test – Plate incorporation procedure

Species/Strain	*S. typhimurium*: TA1535, TA1537, TA98, TA100 *E. coli*: WP2uvrA
Metabolic Activation System	S9 fraction from Aroclor 1254 induced rate liver
Concentration Range in Main Test	Test 1 a) With metabolic activation: 62-5000 µg/plate b) Without metabolic activation: 62-5000 µg/plate Test 2 a) With metabolic activation: 125-2000 µg/plate b) Without metabolic activation: 125-2000 µg/plate
Vehicle	Demineralized water
Remarks - Method	Minor modifications were to the method, but no significant protocol deviations. Vehicle and positive controls were conducted concurrently.

RESULTS

Metabolic Activation	*Test Substance Concentration (µg/plate) Resulting in:*			
	*Cytotoxicity in Preliminary Test**	*Cytotoxicity in Main Test*	*Precipitation*	*Genotoxic Effect*
Absent	-			
Test 1		≥ 556	> 5000	negative
Test 2		≥ 1000	> 2000	negative
Present	-			
Test 1		≥ 5000	> 5000	negative
Test 2		≥ 2000	> 2000	negative

* Not conducted

Remarks - Results	Precipitation was not observed at any concentration; however the test concentrations were described by the test authors as being like emulsions. No toxicologically significant increases in the frequency of revertant colonies were recorded for any of the bacterial strains, with any dose of the test material, either with or without metabolic activation. All the positive control chemicals used in the test induced marked increases in the frequency of revertant colonies thus confirming the activity of the S9-mix and the sensitivity of the bacterial strains.
CONCLUSION	The notified polymer was not mutagenic to bacteria under the conditions of the test.
TEST FACILITY	Stockhausen GmbH (2008e)

BIBLIOGRAPHY

Boethling RS & Nabholz JV (1997) Environmental Assessment of Polymers under the U.S. Toxic Substances Control Act. In: Hamilton JD & Sutcliffe R, ed. Ecological Assessment of Polymers; Strategies for product stewardship and regulatory programs. New York, Van Nostrand Reinhold.

NOHSC (2004) Approved Criteria for Classifying Hazardous Substances, 3rd edition [NOHSC:1008(2004)]. National Occupational Health and Safety Commission, Canberra, AusInfo.

NOTOX B.V (2012) Determination of Physico-Chemical Properties of [notified polymer] (Project. No. 498802, October, 2012). The Netherlands, NOTOX B.V. (Unpublished report submitted by the notifier).

Stockhausen GmbH (2008a) Acute Oral Toxicity: Acute – Toxic – Class – Method with the Test Substance [notified polymer] (Final Report No. 182/2008, Study No. 17273, May, 2008). Krefeld, Germany, Stockhausen GmbH (Unpublished report provided by notifier).

Stockhausen GmbH (2008b) Acute Dermal Irritation/Corrosion with the Test Substance [notified polymer] on Rabbits. (Final Report No. 302/2008, Study No. 17280, September, 2008). Krefeld, Germany, Stockhausen GmbH (Unpublished report provided by notifier).

Stockhausen GmbH (2008c) Hen’s Egg Test on the Chorioallantoic Membrane (HET-CAM) with the Test Substance [notified polymer] (Final Report No. 136/2008, Study No. 17273, April, 2008). Krefeld, Germany, Stockhausen GmbH (Unpublished report provided by notifier).

Stockhausen GmbH (2008d) Skin sensitisation with the Test Substance [notified polymer] on Guinea Pigs (Final Report No. 7/2008, Study No. 17168, February, 2008). Krefeld, Germany, Stockhausen GmbH (Unpublished report provided by notifier).

Stockhausen GmbH (2008e) Ames Test on four strains of *Salmonella* Typhimurium and the *Escherichia coli strain* WP2 uvrA with the test substance [notified polymer] (Final Report No. 79/2008, Study No. 17270, July, 2008). Krefeld, Germany, Stockhausen GmbH (Unpublished report provided by notifier).

SWA (2012) Code of Practice: Managing Risks of Hazardous Chemicals in the Workplace, Safe Work Australia, http://www.safeworkaustralia.gov.au/sites/swa/about/publications/pages/managing-risks-of-hazardous-chemicals-in-the-workplace.

United Nations (2009) Globally Harmonised System of Classification and Labelling of Chemicals (GHS), 3rd revised edition. United Nations Economic Commission for Europe (UN/ECE), <http://www.unece.org/trans/danger/publi/ghs/ghs_rev03/03files_e.html>.