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NATIONAL INDUSTRIAL CHEMICALS NOTIFICATION AND ASSESSMENT SCHEME (NICNAS)

FULL PUBLIC REPORT

Abil Soft AF 100
(PEG/PPG-7/3 Aminopropyl Dimethicone)

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

For the purposes of subsection 78(1) of the Act, this Full Public Report may be inspected at our NICNAS office by appointment only at 334-336 Illawarra Road, Marrickville NSW 2204.

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

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Director
NICNAS

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1. APPLICANT AND NOTIFICATION DETAILS

APPLICANT(S)
Salkat Australia Pty Ltd (ABN: 30 318 540 786)
262 Highett Rd, HIGHETT VIC 3190

NOTIFICATION CATEGORY
Limited: Synthetic polymer with NAMW ≥ 1000.

EXEMPT INFORMATION (SECTION 75 OF THE ACT)
Data items and details claimed exempt from publication:
Molecular and Structural formulae, Molecular weight, Polymer constituents, Residual Monomers/Impurities, Use Details and Import Volumes.

VARIATION OF DATA REQUIREMENTS (SECTION 24 OF THE ACT)
No variation to the schedule of data requirements is claimed.

2. IDENTITY OF CHEMICAL

CHEMICAL NAME
Siloxanes and Silicones, 3-aminopropyl Me, di-Me, 3-hydroxypropyl Me, ethers with polyethylene-polypropylene glycol mono-Me ether, citrates (salts)

MARKETING NAME(S)
Abil Soft AF100

OTHER NAME(S)
Abil Soft 100 N, K5229 N, Polyether-amino-siloxane in neutralised form.
PEG/PPG-7/3 Aminopropyl Dimethicone (INCI name)

CAS NUMBER
298211-68-4

MOLECULAR WEIGHT
Mn >1000 Da

ANALYTICAL DATA
Reference ^{1}H-, ^{13}C- and ^{29}Si- NMR, IR, GPC spectra were provided.

3. COMPOSITION

DEGREE OF PURITY >50%

4. PHYSICAL AND CHEMICAL PROPERTIES

Tests were performed on commercial product >50% purity.
APPEARANCE AT 20°C AND 101.3 kPa: Colourless to yellowish liquid.

Property	Value	Data Source/Justification
Melting Point	-61°C	Measured.
Boiling Point	Not determined	The notified polymer decomposed at >175°C.

Density	1020 kg/m^3 at °C	Measured.
Vapour Pressure	<1.47 X 10^{-6} kPa at 25°C (or 20°C)	Estimated.
Water Solubility	≤ 6.8 x 10^{-3} g/L at 20°C	Measured.
Hydrolysis as a Function of pH	Not determined	Not able to be determined due to low solubility in water.
Partition Coefficient (n-octanol/water)	log Pow ≥ 5.2.at 20°C	Estimated.
Adsorption/Desorption	log K_{oc} ≥ 4.3	Estimated.
Dissociation Constant	pKa = 2.84, 4.01, 4.90, 17.47 (anionic) 10.20 (cationic)	Estimated.
Particle Size	Not applicable	Notified polymer is a liquid.
Flash Point	91°C at 101.3 kPa	Measured
Flammability in contact with water	Notified polymer not expected to be flammable but impurity may liberate ethanol.	Estimated.
Autoignition Temperature	365°C	Measured.
Explosive Properties	Not expected to be explosive but impurity may be.	Statement by notifier.

DISCUSSION OF PROPERTIES

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

Reactivity

The notified polymer is expected to be stable in water and air under normal conditions of temperature and pressure.The notified polymer is considered to be chemically stable as the silicone is covalently bound to oxygen and/or carbon. However, the impurity is expected to hydrolyse readily in contact with water, resulting in the liberation of ethanol. The amount of ethanol generated is expected to be small and not to result in a flammability hazard.

5. INTRODUCTION AND USE INFORMATION

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

The notified polymer will be imported in 50kg plastic pails.

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

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

PORT OF ENTRY:

SYDNEY

IDENTITY OF MANUFACTURER/RECIPIENTS

The notified polymer will be formulated in suburban Sydney.

TRANSPORTATION AND PACKAGING

The notified polymer will be imported into Australia in 50kg plastic pails as part of a mixed Full Container Load containing other substances. The notified polymer will be stored at the notifier's warehouse prior to transportation to customer sites by truck where it will be formulated into the finished product at <1% and decanted into 300mL and 400mL plastic bottles. The finished product containing the notified polymer will be transported to retail outlets in boxes.

USE

Additive in hair care products at <1%.

OPERATION DESCRIPTION

The notified polymer will be imported in 50kg plastic pails.

The notified polymer is weighed into drums at a dispensary. When required for formulation, the notified polymer is transported to the formulation area, and is manually added from tapped drums to the batch being formulated. Formulation takes place in an open tank with a lid covering 10-30% of the area of the top of the tank.

Upon completion of formulation the batch is transferred by pump into 1000 L Intermediate Bulk Containers (IBC).

The finished product containing <1% of the notified polymer is then automatically filled into 300mL-400mL plastic bottles for retail sale.

6. HUMAN HEALTH IMPLICATIONS

6.1 Exposure assessment

6.1.1 Occupational exposure

NUMBER AND CATEGORY OF WORKERS

Category of Worker	*Number*	*Exposure Duration*	*Exposure Frequency*
Transportation and Storage Staff	1	1 hour per day	6 days per year
QC Sampler	1	1 hour per day	6 days per year
Laboratory Analyst	1	1 hour per day	6 days per year
Dispensary workers	4	1 hour per day	20 days per year
Formulation workers	4	1 hour per day	20 days per year

EXPOSURE DETAILS

Transport and Storage

Waterfront, transport and warehouse workers are not expected to be exposed to the notified polymer except in the event of a spill due to an accident or leaking pail.

QC Sampler and Laboratory Analyst

Dermal, inhalation and ocular exposure to the notified polymer is possible during testing and sampling by QC workers and laboratory analysts. Exposure is minimised by conducting tests in a forced ventilation extraction booth and by workers wearing safety glasses, protective gloves and shoes.

Dispensary and Formulation Workers

At customer facilities dispensary and formulation workers may be exposed to the notified polymer during handling of the pail, pouring the notified polymer into the dispensary for weighing and adding the notified polymer to the blending tank for formulation. Dermal, inhalation and ocular exposure are likely to be the main routes of exposure. However, exposure is expected to be minimised by local exhaust ventilation, safety glasses, protective clothing, shoes and gloves.

Dermal, inhalation and ocular exposure to the notified polymer at <1% in the finished product is also possible during cleaning of the reaction vessel, disconnecting hoses from the reaction vessel to the intermediate bulk containers and cleaning the intermediate bulk containers. Exposure will be minimised by use of safety glasses, protective clothing and gloves.

Workers may also be exposed to small amounts of ethanol generated when the notified polymer is added to aqueous solutions. Significant exposure is not expected because the proportion of notified polymer in the products is low.

End use

There is potential for finished products containing <1% of the notified polymer to be used occupationally, for example, by hairdressers applying hair care products.

6.1.2. Public exposure

The notified polymer will be used in the formulation of hair care products available to the general public.
Public exposure will be widespread and will result through the use of hair care products containing <1% notified polymer. Members of the public will make dermal contact and possibly accidental ocular contact with products containing the notified polymer.

Typical use information is as follows (SSCNFP 2003):

Product	Grams/application	Use frequency (applications per day)	Total dermal exposure (Grams per day)
Hair shampoo	8.0	1	8.0
Hair conditioner	14.0	0.28	3.9

Since the hair care product will be stored and used in a domestic environment, there is the possibility of accidental ingestion by a child.

Public exposure during transport, storage and retail distribution is unlikely unless the packaging is breached.

6.2. Human health effects assessment

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

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

Only limited toxicological data is available on the notified polymer. Skin absorption is not expected to occur, because of the high molecular weight.

The notified polymer is of low acute oral toxicity in a rat study and has an LD_{50} of >2000 mg/kg bw.

There was evidence of slight irritation in the *in vitro* eye irritation test (HET-CAM). This is consistent with the cationic nature of the notified polymer, however it is not classified as an eye irritant based on the test result. However, the potential for eye irritation cannot be ruled out. It is noted that the HET-CAM has not yet been validated for identifying mild to moderate ocular effects, and was not fully supported in a validation trial of chemicals causing severe irritation or corrosion (ICCVAM 2006).

There was no evidence of skin sensitisation in the maximisation test in guinea pigs.

The notified polymer tested negative for mutagenicity in an Ames bacterial reverse mutation study; however, this is not considered sufficient evidence to conclusively state that it would be non-mutagenic to humans.

No data for the notified polymer was submitted on other endpoints.

The notified polymer contains a significant impurity which may react with water to liberate ethanol.
The impurity may also be of concern for inhalation toxicity (US EPA 2002). The degree of concern depends on the relative abundance of lower molecular weight species, but there is no molecular weight threshold above which there would be no concern (US EPA, 2002). The percentage of low molecular weight species in the notified polymer is very low. Therefore the inhalation toxicity hazard is assumed to be low.

Based on the available data the notified polymer is not classified as hazardous under the *Approved Criteria for Classifying Hazardous Substances* (NOHSC, 2004).

6.3. Human health risk characterisation

6.3.1. Occupational health and safety

Only limited toxicological information is available on the notified polymer. The notified polymer is expected to exhibit low acute toxicity, with slight potential for eye irritation based on the HET-CAM test. The reactive impurity has potential for inhalation toxicity and is expected to release ethanol when incorporated in the aqueous formulations. However, the percentage of low molecular weight species is very low and the molecular weight of the impurity is high. Therefore the potential for inhalation toxicity is expected to be low.

The anticipated worker exposure to the notified polymer is expected to be limited, as little direct handling occurs. Exposure is likely during QC sampling and analysis, weighing of the notified polymer into the reaction vessel and cleaning of the reaction vessels and pump lines. Once the polymer has been incorporated in the formulation, exposure would be reduced due to dilution. The impurity would not be present in the formulation once it releases ethanol, however it is not known how quickly this reaction would occur.

Exposure during handling and formulation is expected to be mitigated through the use of engineering controls, such as local exhaust ventilation and personal protective equipment. Therefore, the risk to workers from use of the liquid notified polymer is expected to be acceptable. The risk for hairdressers using the notified polymer in finished hair products is expected to be low due to its low concentration in the product (<1%), its low percentage of low molecular weight species and low hazard.

6.3.2. Public health

The limited data available on the health effects of the notified polymer indicate a low hazard. The public will be exposed to the notified polymer on the skin, eye, scalp or by inhalation at concentrations of <1%. However, the notified polymer should not be absorbed due to its high molecular weight and low levels of low molecular weight species. The reactive impurity is not expected to be present in finished products used by the public. The potential for eye irritation from use of hair products containing the notified polymer should be significantly reduced by the low concentration in use (<1%). Therefore, the risk presented by the notified polymer to the public is considered acceptable.

7. ENVIRONMENTAL IMPLICATIONS

7.1. Environmental Exposure & Fate Assessment

7.1.1 Environmental Exposure

RELEASE OF CHEMICAL AT SITE

As the notified polymer will not be manufactured in Australia, environmental release will not occur during this stage of its lifecycle. The notified polymer will be imported in 50 kg plastic pails and after storage, will be mixed with other ingredients to form the end-use formulated products. It is expected that residual within the import containers will account for <1% and will be disposed of to landfill. A further 1% may be released to trade waste sewer as a result of cleaning mixing equipment.

RELEASE OF CHEMICAL FROM USE

The notified polymer will be formulated as a component of hair care products retailed in 300-400 mL containers. Apart from the estimated <2% residual notified polymer remaining in consumer packaging, which is expected to be disposed of to domestic landfill, the remainder will be washed into the domestic sewer after use.

RELEASE OF CHEMICAL FROM DISPOSAL

Notified polymer released to landfill is expected to be immobile based on its low water solubility, and should associate with soil and organic fractions with the landfill environment. Over time the notified polymer is expected to degrade via biotic and abiotic processes to form simple organic and silicon based compounds.

Notified polymer released to domestic sewer is expected to partition to soil and sediment, based on the log P_{OW} and log K_{OC} values. A proportion of the total volume of notified polymer entering the sewer may be removed in STPs, and will be disposed of to landfill, or to land as fertiliser.

7.1.2 Environmental fate

No environmental fate data were submitted.

7.1.3 Predicted Environmental Concentration (PEC)

Since the majority of the total volume of notified polymer will be released to sewer after use, as a worst case scenario, with no removal within STPs, the PEC has been calculated as follows.

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)	20.496	million
Removal within STP	0%	
Daily effluent production:	4,099	ML
Dilution Factor - River	1.0	
Dilution Factor - Ocean	10.0	
PEC - River:	0.67	µg/L
PEC - Ocean:	0.07	µg/L

Using the Environment Australia (2003) Model incorporating the SimpleTreat model, and assuming no degradation, given the lack of biodegradation values, indicates that 60% may partition to sludge, and 1% volatilisation, with the balance (39%) remaining in effluent. Using this data, a mitigated PEC has been calculated as follows:

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)	20.496	Million
Removal within STP	61%	**Mitigation**
Daily effluent production:	4,099	ML
Dilution Factor - River	1.0	
Dilution Factor - Ocean	10.0	
PEC - River:	0.26	µg/L
PEC - Ocean:	0.03	µg/L

Partitioning to biosolids in STPs Australia-wide may result in an average biosolids concentration of 4.01 mg/kg (dry wt). Biosolids are applied to agricultural soils, with an assumed average rate of 10 t/ha/year. Assuming a soil bulk density of 1000 kg/m^3 and a soil-mixing zone of 0.1 m, the concentration of the notified chemical may approximate 0.04 mg/kg in applied soil. This assumes that degradation of the notified chemical occurs in the soil within 1 year from application. Assuming accumulation of the notified chemical in soil for 5 and 10 years under repeated biosolids application, the concentration of notified chemical in the applied soil in 5 and 10 years may approximate 0.2 mg/kg and 0.4 mg/kg, respectively.

STP effluent re-use for irrigation occurs throughout Australia. The agricultural irrigation application rate is assumed to be 1000 L/m^2/year (10 ML/ha/year). The notified chemical in this volume is assumed to infiltrate and accumulate in the top 0.1 m of soil (density 1000 kg/m^3). Using these assumptions, irrigation with a concentration of 0.261 mg/L may potentially result in a soil concentration of approximately 2.610 x 10^{-3} mg/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 1.305 x 10^{-2} mg/kg and 2.610 x 10^{-2} mg/kg, respectively.

7.2. Environmental effects assessment

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

Endpoint	*Result*	*Assessment Conclusion*
Fish Toxicity	LC50 6.8 mg/L	Toxic to fish.
Daphnia Toxicity	E_iC50 2.53 mg/L	Toxic to aquatic invertebrates.
Algal Toxicity	E_rC50 13.1 mg/L	Harmful to algae.

7.2.1 Predicted No-Effect Concentration

Using the most sensitive endpoint from the ecotoxicity tests presented, the PNEC has been calculated as follows.

Predicted No-Effect Concentration (PNEC) for the Aquatic Compartment		
EC50 (Invertebrates).	2.53	mg/L
Assessment Factor	100.00	
PNEC:	25.30	µg/L

7.3. Environmental risk assessment

Based on the unmitigated PEC and the PNEC calculated above, the risk quotient has been calculated as follows.

Risk Assessment	***PEC µg/L***	***PNEC µg/L***	***Q***
Q - River:	0.67	25.3	0.026
Q - Ocean:	0.07	25.3	0.003

As the Q value is below 1, the risk to the aquatic environment under the proposed volume and use pattern is considered acceptable.

8. CONCLUSIONS AND REGULATORY OBLIGATIONS

Hazard classification

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

and

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

	Hazard category	***Hazard statement***
Environment	Acute II	Toxic to the aquatic environment.
	Chronic II	Toxic to the aquatic environment with long-lasting effects.

Human health risk assessment

Under the conditions of the occupational settings described, the risk to workers is considered to be acceptable.

When used in the proposed manner the risk to the public is considered to be acceptable.

Environmental risk assessment

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

Recommendations

REGULATORY CONTROLS

CONTROL MEASURES
Occupational Health and Safety

- Employers should implement the following engineering controls to minimise occupational exposure to the notified polymer as introduced:
  - Local exhaust ventilation.

- Employers should implement the following safe work practices to minimise occupational exposure during handling of the notified polymer as introduced:
  - Avoid contact with eyes.
  - Prevent aerosol formation.
  - Avoid inhalation.

- Employers should ensure that the following personal protective equipment is used by workers to minimise occupational exposure to the notified polymer as introduced:
  - Gloves.
  - Safety goggles.
  - Respiratory protection where appropriate.
  - Protective clothing.

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

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

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

Disposal

- The notified chemical should be disposed of to landfill.

Emergency procedures

- Spills or accidental release of the notified chemical should be handled by physical containment, collection and subsequent safe disposal.
- The MSDS for the notified polymer should note that flammable gas may be generated.

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(2) of the Act; if

- the function or use of the polymer has changed from additive in hair product at <1%, or is likely to change significantly;
- the amount of polymer being introduced has increased from 1 tonne, or is likely to increase, significantly;
- if 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.

No additional secondary notification conditions are stipulated.

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

APPENDIX A: PHYSICAL AND CHEMICAL PROPERTIES

Melting Point -61°C

Method	OECD TG 102 Melting Point/Melting Range. EC Directive 92/69/EEC A.1 Melting/Freezing Temperature.
Remarks	Differential Scanning Calorimetry (DSC) was used.
Test Facility	Notox B.V., s-Hertogenbosch, The Netherlands (2007)

Boiling Point Decomposed without boiling

Method	OECD TG 103 Boiling Point. EC Directive 92/69/EEC A.2 Boiling Temperature.
Remarks	IN a DSC test, reaction and/or decomposition of the notified chemical were observed above approximately 175°C; boiling of the chemical was not observed below the temperature at which reaction and/or decomposition started. Therefore the notified chemical has no boiling temperature.
Test Facility	Notox B.V., s-Hertogenbosch, The Netherlands (2007)

Density 1020 kg/m^3

Method	OECD TG 109 Density of Liquids and Solids. EC Directive 92/69/EEC A.3 Relative Density.
Remarks	Pycnometer method.
Test Facility	Notox B.V., s-Hertogenbosch, The Netherlands (2007)

Vapour Pressure $<1.47 \times 10^{-6}$ kPa at 25°C (estimated).

Method	OECD TG 104 Vapour Pressure. EC Directive 92/69/EEC A.4 Vapour Pressure.
Remarks	It was found that the notified chemical reacted and/or decomposed at a temperature above 175°C. The results of the test were therefore compared with the results of hexachlorobenzene. The weight loss of the test substance at 140°C was lower than the weight loss of hexachlorobenzene at the same temperature. From this, it was concluded that the vapour pressure of the notified chemical was $<1.47 \times 10^{-3}$ Pa.
Test Facility	Notox B.V., s-Hertogenbosch, The Netherlands (2007)

Water Solubility $\leq 6.8 \times 10^{-3}$ g/L at 20°C

Method	OECD TG 105 Water Solubility. EC Directive 92/69/EEC A.6 Water Solubility.
Remarks	Flask Method. The test substance was stirred with double distilled water at nominal concentrations between 1.21 and 110 mg/L at 19.8±0.7°C for 71.3 hours. Since a sensitive analytical method was not available, the test sample was visually interpreted after stirring. The presence of undissolved test substance was confirmed by examination for the Tyndall effect using a single-beam UV-Vis spectrophotometer between 190 and 800 nm. The spectra showed, that even the lowest concentration level tested, generates an increase of the baseline as compared to a blank solution. In order to give an estimate of the water solubility of the test substance, the absorbance at 800 nm was determined and related to the limit of detection. The test substance was considered water soluble at all concentration levels with absorption below the LOD.
Test Facility	Notox B.V., s-Hertogenbosch, The Netherlands (2007)

Hydrolysis as a Function of pH Not determined

Remarks	The water solubility was determined to be ≤6.80 mg/L. Since a sensitive analytical method to support the hydrolysis test at such low concentration levels was not available, the hydrolysis test could not be performed. The notified chemical does not contain

hydrolysable functionality.

Test Facility Notox B.V., s-Hertogenbosch, The Netherlands (2007)

Partition Coefficient (n-octanol/water) log Pow ≥ 5.2.at 20°C

Method OECD TG 117 Partition Coefficient (n-octanol/water).
EC Directive 92/69/EEC A.8 Partition Coefficient.

Remarks Estimation Method. Test substance was stirred with n-octanol at a nominal concentration of 1.13 x 10^3 g/L at 19.6±0.2°C for 3 hours. After stirring, the test substance was determined to be miscible with n-octanol in at least 1:1 (w/v) ratio by visual observation. The P_{OW} was determined using the quotient of this and the water solubility.

Test Facility Notox B.V., s-Hertogenbosch, The Netherlands (2007)

Adsorption/Desorption log K_{oc} ≥ 4.3

Method OECD TG 121 Adsorption - Desorption Using HPLC.

Remarks Due to the nature of the test substance, it was not possible to determine the K_{OC} value of the test substance using the HPLC method, the QSAR calculation method was applied. Based on the water solubility of the test substance, the compound was classified as "predominantly hydrophobic". For this chemical class, the log K_{OC} was derived using the following formula: log K_{OC} = 0.81logP_{OW} + 0.10.

Test Facility Notox B.V., s-Hertogenbosch, The Netherlands (2007)

Dissociation Constant pKa = 2.84, 4.01, 4.90, 17.47 (anionic) 10.20 (cationic)

Method OECD TG 112 Dissociation Constants in Water.

Remarks It proved not possible to determine the pK_a values of the test substance experimentally. Therefore, the pK_a values were calculated using the pKalc ver. 5.0 computer program.

Test Facility Notox B.V., s-Hertogenbosch, The Netherlands (2007)

Particle Size Not applicable

Remarks Not measured as the notified chemical is a liquid.

Flash Point 91°C at 101.3 kPa

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

Remarks Pensky-Martens Closed Cup Tester was used.

Test Facility Notox B.V., s-Hertogenbosch, The Netherlands (2007)

Flammability in contact with water Not determined.

Remarks The structure of the notified polymer does not contain groups that might lead to the evolution of a dangerous amount of flammable gas when coming into contact with water or damp air. The polymer is considered to be chemically stable as the silicone is covalently bound to oxygen and/or carbon and there are no metals, transition metals or boron present. However, the impurity, present in a significant quantity, may hydrolyse upon contact with water liberating ethanol.

Autoignition Temperature 365°C

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

Remarks

Test Facility Notox B.V., s-Hertogenbosch, The Netherlands (2007)

Explosive Properties

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

Remarks The molecular structure of the notified polymer does not contain any chemically unstable or highly energetic groups that might lead to an explosion. The oxygen balance could not be determined because the exact structure is unknown.

Test Facility	Notox B.V., s-Hertogenbosch, The Netherlands (2007)

Surface Tension Not determined.

Method	OECD TG 115 Surface Tension of Aqueous Solutions. EC Directive 92/69/EEC A.5 Surface Tension.
Remarks	The water solubility was determined to be ≤6.80 mg/L. At this concentration undissolved matter is still present. Therefore the surface tension test was not performed.
Test Facility	Notox B.V., s-Hertogenbosch, The Netherlands (2007)

APPENDIX B: TOXICOLOGICAL INVESTIGATIONS

B.1. Acute toxicity – oral

TEST SUBSTANCE	Notified chemical (liquid).
METHOD	OECD TG 423 Acute Oral Toxicity – Acute Toxic Class Method. EC Directive 92/69/EEC B.1tris Acute Oral Toxicity – Acute Toxic Class Method.
Species/Strain	Rat/Wistar
Vehicle	Test substance administered as supplied.
Remarks - Method	No significant protocol deviations.

RESULTS

Group	*Number and Sex of Animals*	*Dose mg/kg bw*	*Mortality*
I	3 per sex	200	0/6
II	3 per sex	2000	0/6

LD50	>2000 mg/kg bw
Signs of Toxicity	Slightly increased salivation was observed in 2 out of 3 rats in Group II, 10 mins after administration. Breathing sounds were observed in one animal out of 3 males and 3 females in Group II, between 1hr and 4hrs after administration.
Effects in Organs	There were no remarkable necropsy findings.
Remarks - Results	200 mg/kg bw was administered to 3 males and 3 females in Group I. Since no mortality was observed within some days, 2000 mg/kg was administered to 3 male rats (Group II). Since no mortality was observed within some days, 2000 mg/kg bw was administered to 3 female rats (Group II).
CONCLUSION	The notified chemical is of low toxicity via the oral route.
TEST FACILITY	Harlan Bioservice for Science GmbH (2000a)

B.2. Skin sensitisation

TEST SUBSTANCE	Notified chemical (liquid).
METHOD	OECD TG 406 Skin Sensitisation - Maximization Test in Guinea Pigs. EC Directive 96/54/EC B.6 Skin Sensitisation – Maximization Test in Guinea Pigs.
Species/Strain	Guinea pig/Pirbright White
PRELIMINARY STUDY	Maximum Non-irritating Concentration: intradermal: 0.1% topical: 100%
MAIN STUDY	
Number of Animals	Test Group: 10 Control Group: 5
INDUCTION PHASE	Induction Concentration: Intradermal injection: 0.1% Topical application: Undiluted.
Signs of Irritation	Intradermal injection: No signs of irritation were observed in test or control animals after intradermal injection. Topical application: The test sites were pre-treated with 10% sodium lauryl sulphate 24-hours before topical induction. No erythema was observed in test or control animals following topical induction.
CHALLENGE PHASE	
1st challenge	topical: Test substance as supplied.
Remarks - Method	

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	Undiluted.	0/10	0/10	-	-
Control Group	Undiluted.	0/5	0/5	-	-

Remarks - Results

CONCLUSION There was no evidence of reactions indicative of skin sensitisation to the notified chemical under the conditions of the test.

TEST FACILITY Harlan Bioservice for Science GmbH (2000b).

B.3. Hen's Egg Test - Chorioallantoic Membrane (HET-CAM) Test for Eye Irritation Potential

TEST SUBSTANCE Notified chemical (liquid).

METHOD Test conducted according to HET-CAM Method. Ref. Steiling, W. (1999) Eggs from White Leghorn hens were incubated for nine days (blunt end upwards). On day 10, their blunt ends were illuminated with a candling lamp. During candling the air space outlined at the blunt end of the eggs was marked. The marked section of the shell is removed and the white egg membrane moistened with physiological saline.

The chorioallantoic membranes of two eggs were used to test the positive control (Texapon ASV 5%) and the notified chemical. 300µL of the notified substance was applied to each membrane. After 30 seconds, the test item was rinsed off the membrane with physiological saline. Each membrane was assessed for haemorrhage, lysis or coagulation effects and scored from 0 (no reaction) to 3 (strong reaction).

Evaluation The irritation classification is based on the effect with the highest score.

The method in the Main Test was identical to the Preliminary Test using the chorioallantoic membranes of 6 eggs each for the notified substance and the positive control (Texapon ASV 5%).

RESULTS

Group	*Type of Reaction*				
	Haemorrhage	Lysis	Coagulation	Irritation value Score	Irritation classification
Notified chemical	3	0	0	3	Slightly irritating
Positive control	11	9	0	11	Moderately irritating

Remarks - Results The notified chemical induced slight haemorrhaging in 3 of the 6 membranes. Irritation classification: slightly irritating (<6).
The positive control induced slight to moderate haemorrhaging and slight to moderate lysis in all 6 membranes. Irritation classification: moderately irritating (≥6 and <12).

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

TEST FACILITY L+S AG (2005)

B.4. Genotoxicity – bacteria

TEST SUBSTANCE	Notified chemical (liquid).
METHOD	OECD TG 471 Bacterial Reverse Mutation Test. EC Directive 92/35/EC B.13/14 Mutagenicity – Reverse Mutation Test using Bacteria. Plate incorporation procedure/Pre incubation procedure
Species/Strain	*S. typhimurium*: TA1535, TA1537, TA98, TA100. *E. coli*: WP2uvrA (pKM101).
Metabolic Activation System	S9 fraction from Phenobarbital/β-naphtoflavone induced rat liver.
Concentration Range in Main Test	a) With metabolic activation: 0.05 – 5.0 µL/plate b) Without metabolic activation: 0.05 – 5.0 µL/plate
Vehicle	Test substance administered as supplied.
Remarks - Method	No significant protocol deviations.

RESULTS

Metabolic Activation	*Test Substance Concentration (µl/plate) Resulting in:*			
	Cytotoxicity in Preliminary Test	*Cytotoxicity in Main Test*	*Precipitation*	*Genotoxic Effect*
Absent				
Test 1	>5	>5	>5	Negative
Test 2	>5	>5	>5	Negative
Present				
Test 1	>5	>5	>5	Negative
Test 2	>5	>5	>5	Negative

Remarks - Results

CONCLUSION	The notified chemical was not mutagenic to bacteria under the conditions of the test.
TEST FACILITY	L+S AG (2000)

APPENDIX C: ENVIRONMENTAL FATE AND ECOTOXICOLOGICAL INVESTIGATIONS

C.1. Ecotoxicological Investigations

C.2.1. Acute toxicity to fish

TEST SUBSTANCE	Notified polymer.
METHOD	OECD TG 203 Fish, Acute Toxicity Test –Static.
Species	Zebra Fish (*Brachydanio rerio*)
Exposure Period	96 h
Auxiliary Solvent	Nil
Water Hardness	40-180 mg $CaCO_3$/L
Analytical Monitoring	DOC
Remarks – Method	Based on the results of preliminary range finding tests, the study was performed with 5 concentration levels ranged from 1 to 16 mg/L in a geometrical series with a dilution factor of 2. These were prepared by directly weighing and mixing in a laboratory blender (20000 rpm, 1 minute). LC50 values and confidence intervals were calculated by probit analysis.

RESULTS

Concentration mg/L		*Number of Fish*	*Mortality*			
Nominal	*Actual*		*24 h*	*48 h*	*72 h*	*96 h*
0		7	0	0	0	0
1		7	0	0	0	0
2		7	0	0	0	0
4		7	0	0	0	0
8		7	2	5	6	6
16		7	7	7	7	7

LC50	6.8 mg/L at 96 hours. 95% CI = 6.2 – 7.6. (Nominal Concentration)
NOEC	4.0 mg/L at 96 hours. (Nominal Concentration)
Remarks – Results	Concentration control analysis was carried out only at test start according to the sponsor's wish. Therefore, no information on stability and recovery of the test item under test conditions was given. Due to the low carbon content of the test item, only the highest concentration level of 16 mg/L was analytically verified via analysis of dissolved organic carbon. Therefore the results are reported in terms of nominal concentration only. Water quality parameters of temperature, pH, O_2 Saturation measured at 0, 24, 48, 72 and 96 h were determined to be within acceptable limits. After 72 h of exposure, 0.5 mL aliquots of the test medium from the nominal test concentrations of 4 – 16 mg/L and control were transferred to 10 mL untreated test medium. Algae were then allowed to grow further 3 days under test conditions. From initial and final cell density, it was determined that when previously exposed cells are placed in clean medium, growth is no longer inhibited. Therefore, there is potential for recovery following exposure at 16 mg/L, the highest concentration tested.
CONCLUSION	The notified chemical is toxic to Zebra Fish.
TEST FACILITY	Dr.U.Noack-Laboratorium (2001a)

C.2.2. Acute toxicity to aquatic invertebrates

TEST SUBSTANCE	Notified polymer.
METHOD	OECD TG 202 Daphnia sp. Acute Immobilisation Test and Reproduction Test – Static. EC Directive 92/69/EEC C.2 Acute Toxicity for Daphnia - Static.
Species	*Daphnia magna*
Exposure Period	48 hours
Auxiliary Solvent	Nil
Water Hardness	160-180 mg $CaCO_3$/L
Analytical Monitoring	DOC
Remarks - Method	Based on the results of a preliminary test, a definitive test was performed with 5 concentrations of a 10 mg/L stock solution ranging from 1.0 to 10 mg/L with a dilution factor of 1.8 to enable the determination of 0 and 100% immobilisation after 24 and 48 hours. The reference item potassium dichromate was used to validate the study.

RESULTS

Concentration mg/L		*Number of D. magna*	*Number Immobilised*	
Nominal	*Actual*		*24 h*	*48 h*
0	-	20	0	0
1	-	20	0	0
1.8	-	20	0	2
3.2	0.92	20	6	15
5.8	1.79	20	20	20
10	2.77	20	20	20

E_iC50	2.53 mg/L at 48 hours. 95% CI: 2.32-2.75. (Nominal Concentration)
NOE_iC	1 mg/L at 48 hours. (Nominal Concentration)
Remarks - Results	DOC was measured in all concentration levels and control at the start of the test. The test item was only analytically verified at the beginning of the test due to the sponsor's wish. The test item solutions were clearly dissolved in all tested concentration levels throughout exposure.
CONCLUSION	The notified polymer is toxic to *Daphnia magna*.
TEST FACILITY	Dr.U.Noack-Laboratorium (2001b)

C.2.3. Algal growth inhibition test

TEST SUBSTANCE	Notified polymer.
METHOD	OECD TG 201 Alga, Growth Inhibition Test. EC Directive 92/69/EEC C.3 Algal Inhibition Test.
Species	*Desmodesmus subspicatus*
Exposure Period	72 hours
Concentration Range	Nominal: 0.125, 0.25, 0.5, 1, 2, 4, 8 and 16 mg/L Actual: … mg/L
Auxiliary Solvent	Nil
Analytical Monitoring	DOC
Remarks - Method	The reference item Potassium dichromate was used to validate the test. The E_bC_{50} and E_rC_{50} values and confidence intervals after 72 h analyses were calculated by probit analysis. The NOE_bC and NOE_rC were determined by calculation of statistical significance of biomass integrals and growth rates. No significant deviations from the test protocol were reported.

RESULTS

Biomass		*Growth*	
E_bC_{50} mg/L at 72 h	*NOE_bC mg/L*	*E_rC_{50} mg/L at 72 h*	*NOE_rC mg/L*
2.95 95% CI: 2.56-3.40	0.5	13.1 95% CI: 10.7-16.0	1

Remarks - Results	Results are reported for nominal concentrations only. The study met the validity criteria of the guideline.
CONCLUSION	The notified polymer is harmful to *Desmodesmus subspicatus*.
TEST FACILITY	Dr.U.Noack-Laboratorium (2004)

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