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**NATIONAL INDUSTRIAL CHEMICALS NOTIFICATION  
AND ASSESSMENT SCHEME**

**FULL PUBLIC REPORT**

**Siloxanes and silicones, di Me, 3-[3-[(3-cocoaminopropyl)  
dimethylammonio] 2-hydroxypropoxy] propyl group terminated,  
acetates (salts)**

This Assessment has been compiled in accordance with the provisions of the *Industrial Chemicals (Notification and Assessment) Act 1989*, as amended and Regulations. This legislation is an Act of the Commonwealth of Australia. The National Industrial Chemicals Notification and Assessment Scheme (NICNAS) is administered by Worksafe Australia which also conducts the occupational health & safety assessment. The assessment of environmental hazard is conducted by the Department of the Arts, Sport, the Environment and Territories and the assessment of public health is conducted by the Department of Health, Housing and Community Services.

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Director  
Chemicals Notification and Assessment

**FULL PUBLIC REPORT**

**Siloxanes and silicones, di Me, 3-[3-[(3-cocoaminopropyl) dimethylammonio] 2-hydroxypropoxy] propyl group terminated, acetates (salts)**

**1. APPLICANTS**

International Sales and Marketing Pty Ltd/Salkat Australia Pty Ltd, 262 Highett Rd, Highett, Vic, 3190.

**2. IDENTITY OF THE CHEMICAL**

**Chemical name:** Siloxanes and silicones, di Me, 3-[3-[(3-cocoaminopropyl) dimethylammonio] 2-hydroxypropoxy] propyl group terminated, acetates (salts)

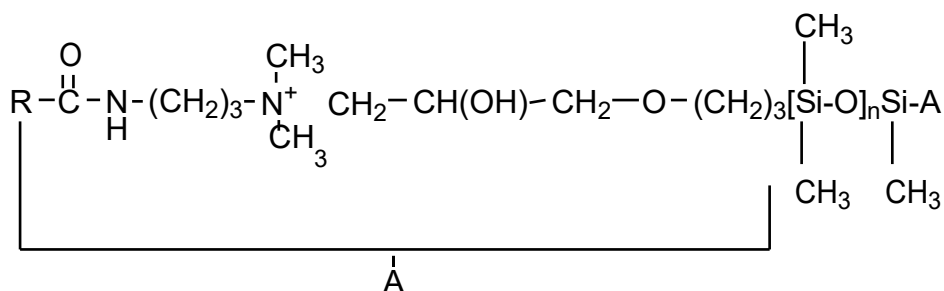
**Chemical Abstracts Service (CAS) Registry No.:** 134737-05-6

**Other names:** Di-quaternised poly di-methylsiloxanespolysiloxanes (CTFA)

**Trade names:** ABIL Quat 3270, ABIL Quat 3272

**Molecular formula:** C<sub>72</sub>H<sub>166</sub>N<sub>4</sub>O<sub>19</sub>Si<sub>10</sub>

**Structural formula:**



n = 9 (ABIL Quat 3270) or 30 (ABIL Quat 3272)  
R =  $CH_3-(CH_2)_x$

**Number-average molecular weight:** ~1670 (ABIL Quat 3270)  
~3200 (ABIL Quat 3272)

**Weight-average molecular weight:**

**Maximum percentage of low  
molecular weight species**

(molecular weight < 1000): none

**Monomers/Reactants:**

Chemical name:	CAS No.:	Weight percentage:
Siloxanes and silocones, di me, 3-(oxiranylmethoxy) propyl group terminated	102782-97-8	57.9
Amide, coco, N-[3- (dimethylammonio) propyl]	68140-01-2	36.2
Acetic acid	64-19-7	5.9

**Method of detection and determination:** Infra-red spectroscopy, nuclear magnetic resonance spectroscopy, gas chromatography and thermal gravimetric analysis.

**Spectral data:** The following spectra were provided for ABIL Quat 3270

An infra-red spectrum with major peaks at 3267, 2961, 2926, 2855, 1653, 1576, 1400, 1260, 1092, 1032 and 802  $\text{cm}^{-1}$ .

A  $^{13}\text{C}$  nuclear magnetic resonance spectrum with chemical shifts occurring at -0.6, 0.3, 0.5, 13.4, 22.0, 22.2, 22.7, 24.0, 25.2, 28.6, 28.8, 28.9, 29.0, 31.2, 35.4, 35.5, 44.6, 51.7, 62.8, 63.4, 72.2, 73.7, 76.7, 77.1, 77.5, 173.7 and 176.6 ppm relative to TMS.

An  $^1\text{H}$  nuclear magnetic resonance spectrum was also provided, however the peak positions were not easily estimated from the scale.

### 3. PHYSICAL AND CHEMICAL PROPERTIES

<b>Appearance at 20°C and 101.3 kPa:</b>	the pure chemical is a highly viscous "liquid salt" trade products are amber liquids
<b>Odour:</b>	the trade products have an aromatic odour {if distinctive}
<b>Glass-transition Temperature:</b>	°C
<b>Viscosity:</b>	~400 $\text{mm}^2\text{s}^{-1}$ (ABIL Quat 3270); ~1000 $\text{mm}^2\text{s}^{-1}$ (ABIL Quat 3272)
<b>Surface Tension:</b>	~31.5 $\text{g/cm}^3$ (ABIL Quat 3270); ~44 $\text{g/cm}^3$ (ABIL Quat 3272) {for density}
<b>Specific Gravity/Density:</b>	~1014 $\text{kg/m}^3$ (ABIL Quat 3270); ~1008 $\text{kg/m}^3$ (ABIL Quat 3272) {for density}
<b>Vapour Pressure:</b>	0.07 mmHg @ 20°C (product)

<b>Water Solubility:</b>	the product is soluble in water; solubility decreasing with increasing degree of polymerisation of the dimethylpolysiloxane moiety g/L at 20°C
<b>Fat Solubility:</b>	
<b>Partition Co-efficient:</b>	
<b>Hydrolysis as a function of pH:</b>	no hydrolysis expected @ pH 4-9  @ pH <2 and >11, and @ >90°C, cleavage of Si-O-Si bonds of dimethylpolysiloxane is expected
<b>Adsorption/Desorption:</b>	
<b>Dissociation Constant:</b>	expected to dissociate completely
<b>Flash Point:</b>	90 °C for trade products
<b>Flammability Limits:</b>	
<b>Oxidation Products:</b>	at high temperatures the trade products oxidise giving rise to propionaldehyde, lactic acid, pyruvic acid and acetic acid.
<b>Reactivity/Stability:</b>	there is no specific reactivity

Methods to estimate melting and boiling point are not applicable as the notified polymer is a high viscous liquid.

Partition coefficient was not measured due to the salt character of the notified polymer. The polymeric salt is expected to be completely dissociated.

The environmental properties of fluids have been well reviewed by Hamelink (1). Silicone fluids are very surface active because the flexible siloxane linkages permit alignment of the hydrophobic methyl substituents towards the non-polar phase, and of the polysiloxane backbone towards the polar phase. The polar medium is generally water, and apolar media to which polydimethylsiloxanes become attached may be textiles, sewage sludge, hair, algae, sediment etc. In aqueous environments, polydimethylsiloxanes are adsorbed onto sedimenting particles. Also, in the presence of nitrate ions, which exist at various concentrations in the environment, short chain siloxanes are photodegraded to the level of silicate within days (2).

<b>Pyrolysis Products:</b>	-----?
<b>Decomposition Temperature:</b>	not supplied
<b>Decomposition Products:</b>	-----?
<b>Autoignition Temperature:</b>	°C
<b>Explosive Properties:</b>	
<b>Particle size distribution:</b>	range -    µm mean   -    µm
<b>Melting Point/Boiling Point:</b>	°C
<b>Vapour Pressure:</b>	kPa at 25°C
<b>Partition Co-efficient (n-octanol/water)</b>	log P <sub>O/W</sub> :
<b>Adsorption/Desorption:</b>	not measured
<b>Particle size distribution:</b>	range -    µm mean   -    µm
<b>Flammability Limits:</b>	not measured
<b>Autoignition Temperature:</b>	not measured
<b>Explosive Properties:</b>	not measured

#### 4. PURITY OF THE CHEMICAL

**Degree of purity** (of the notified chemical alone): >97%

**Toxic or hazardous impurities:** none

**Non-hazardous impurity/impurities:** none > 1% by weight

**Maximum content of residual monomers/reactants:** 0.3%

**Additive:**

<b>Chemical name:</b>	1,2 propanediol
<b>Synonym:</b>	propylene glycol
<b>CAS No.:</b>	57-55-6
<b>Weight percentage:</b>	~50

#### 5. INDUSTRIAL USE

The notified chemical will initially be imported into Australia at 2000 kg/annum, with possible increases in import volume to meet future markets. The notified polymer will be imported in two formulations, ABIL Quat 3270 and ABIL Quat 3272, each containing 50% of the polymer in propylene glycol. These formulations will be used in the cosmetics industry as shampoo/conditioner components (final polymer concentration up to 2.5%). Abil-Quat 3272 which is of higher molecular weight than Abil-Quat 3270 is more compatible with anionic surfactants than the latter. Therefore, Abil-Quat 3272 is preferred for use in shampoos, shower- and bath preparations and liquid soaps, whereas the most important areas of application for Abil-Quat 3270 are conditioning hair rinses.

Formulations containing the notified polymer may also find applications as ingredients for fabric softeners, corrosion inhibitors, antistatic additives for plastics, pigment dispersants and fibre lubricants (final polymer concentration up to 2%).

#### 6. OCCUPATIONAL EXPOSURE

The notified polymer will be imported in 50 kg drums in the two formulations ABIL Quat 3270 and ABIL Quat 3272. Both imported formulations will contain 50% polymer in ethylene glycol. They

will be transported by road to five manufacturing plants. Workers at these sites will weigh and mix the polymer solutions into shampoo or conditioner formulations, and package the final products for shipment to the end users (wholesalers, hair salons). ABIL Quat 3270 or ABIL Quat 3272 will constitute no more than 5% of shampoos, skin cleansing products or conditioning hair rinses (0.2-2% in shampoos, 0.5-4% in rinses). Other constituents of these products will be anionic surfactants, water insoluble components, solubilizers and pearlizing agents.

Worker exposure will vary at each manufacturing plant. The number of workers exposed to the notified polymer at Wella Australia, Schwarzkopf Pty Ltd, Alf Tooth Enterprises Pty Ltd and Avon Products/Innoxia is estimated at 7, 3, 2 and 2 respectively. It is envisaged that half of the volume of polymer imported will be used by Wella Australia (ie, 1000 kg). The time spent on each task (eg mixing, weighing) will also vary at each site, making an accurate measure of the exposure difficult.

The notifier states that special guidelines and precautions will be used during production such as the use of enclosed systems when splashings or spillages are anticipated and the use of personal protective equipment. The number of workers handling the polymer is not anticipated to be large and most worker contact with the chemical is expected to be low under normal use situations.

Hair salon workers will also be exposed to the notified polymer, however, the concentration of notified polymer will at most be 2.5%.

## **7. PUBLIC EXPOSURE**

The notified polymer is to be imported into Australia as a 50% solution in propylene glycol. It will be transported by road to five clients, where it will be incorporated into shampoo and conditioner products, which will be sold to wholesalers and hair salons, and eventually to the public. The concentration of the notified polymer in shampoos and conditioners will at most be 2.5%.

One of the clients has indicated that disposal of any unspent polymer which is approximated at 8-10 kg/annum will be in the company's waste-water treatment plant. Discharge from the plant



to the sewer is in accordance with Council's discharge specifications. Furthermore, since the substance is to be used in shampoos and conditioners, disposal of the spent products containing the notified polymer will occur in the household and hair salons, probably via the sewage system.

## **8. ENVIRONMENTAL EXPOSURE**

### **. Release**

The notifier has provided information on the production procedures of one of its customers, Cosmetic Products Pty Ltd (trading as Wella). It states they have in place procedures aimed at reducing the level of waste in all areas of operations. The company's factory is equipped with a modern waste water treatment plant (dissolved air flotation with chemical pre-treatment and biological oxidation). Discharge from the plant to sewer is monitored on a regular basis by the company and the Local Council's requirement in regard to the company's discharge specifications. Shampoo waste is currently running at approximately 1.2 - 1.5% of manufactured quantity depending on product's viscosity. The company is aiming to reduce this to below 1% by the end of 1993.

The company estimates that they would be utilising approximately 1000 kg of Abil-Quat 3272 in 1993 to produce 80 to 100 tonnes of finished shampoo products containing the notified substance. This would translate to a maximum of 8 - 10 kg of the notified substance waste being generated in a 12 monthly period by the company prior to treatment.

Waste polymer from the other shampoo/conditioner formulating sites is likely to enter the sewer system.

The polymer will be released to the aquatic environment when consumers wash the polymer residues from their hair.

### **. Fate**

When the polymer enters sewer systems it is likely to be adsorbed to suspended matter and become associated with sludge at wastewater treatment plants. Any polymer that remains in treated waste water and enters receiving waters is likely to be degraded to silicates by photolysis.

Sludge containing the notified substance may be incinerated or landfilled. Incineration would destroy the substance and liberate oxides of carbon, nitrogen and silicon, while disposal to landfill would immobilise it. Polydimethylsiloxanes are thought to be unstable in terrestrial environments, where clays can catalyse cleavage of the siloxane linkage, but are probably more permanent in aquatic sediment as the catalytic action of clays is inversely related to their degree of hydration (1).

The notified substance contains an amide linkage that may be susceptible to hydrolysis. However, hydrolysis of the notified substance is unlikely under environmental conditions due to its hydrolytic stability and expected adsorption to surfaces.

## 9. EVALUATION OF TOXICOLOGICAL DATA

Toxicological data are not required for polymers with number-average molecular weight greater than 1000 under the *Industrial Chemicals (Notification and Assessment) Act 1989 as amended* (the Act). However, studies were conducted using ABIL Quat 3270 and the data submitted for assessment.

### 9.1 Acute Toxicity

Table1 Summary of the acute toxicity of ABIL Quat 3270

Test	Species	Outcome	Reference
Oral	Rat	LD <sub>50</sub> > 5091 mg/kg	1
Skin	Rabbit	non-irritant	2
Eye	Rabbit	non-irritant	3

#### 9.1.1 Oral Toxicity (3)

This study was conducted in accordance with OECD guideline No: 401 (6).

Undiluted ABIL Quat 3270 (5 ml/kg) was administered by stomach tube to 10 Wistar rats (5 male and 5 female). Clinical

observations were made over a 14 day period. All rats were subjected to necropsy. No deaths occurred and all rats showed no clinical or toxicological symptoms over the entire observation period. Upon necropsy at the end of the 14 day observation period, no macroscopic lesions were reported in the cranial, thoracic and abdominal cavity. Bodyweight gains were unaffected by treatment.

Results of this study indicate an acute oral LD<sub>50</sub> of > 5091 mg/kg (equivalent to > 5 ml/kg) in rats of both sexes for ABIL Quat 3270.

#### **9.1.2 Skin Irritation (4)**

This study was conducted in accordance with OECD guideline No: 404 (7).

A single dose of 0.5 ml diluted ABIL Quat 3270 (10% w/w in distilled water) was applied occlusively to the abraded and intact skin of 6 New Zealand white rabbits. Twenty-four hours later, the dressings were removed and the test areas wiped to prevent further exposure. The test sites were evaluated 24 and 72 hours after the initial application. Very slight to well-defined erythema was observed in all animals on both abraided and non-abraided sites 24 hours after dosing. By 72 hours, erythema had decreased in two animals and completely disappeared in a further 3. No oedema was observed at either 24 or 72 hours. All rabbits appeared healthy and active during the test period.

Results of this study indicate that ABIL Quat 3270 is not a skin irritant in rabbits.

#### **9.1.3 Eye Irritation (5)**

This study was conducted in accordance with OECD guideline No: 405 (8).

A single dose of 0.1 ml 3% ABIL Quat 3270 in deionised water was instilled in the conjunctival sac of the left eye of each of 6 New Zealand white rabbits. The right eye served as the control. The treated eyes of 3 animals were washed 4 seconds after application with 10 ml luke warm water. Ocular reactions were assessed at 1, 24, 48 and 72 hours after treatment. Eye lesions were assessed

by means of 1% fluorescein (1 drop/eye) and UV-light for all but the 1 and 48 hour observations. All effects were scored according to Draize (described in 8). There was no evidence of corneal opacity or uveitis in any of the animals over the entire observation period. Erythema of the conjunctiva was observed in all rabbits, and these reactions persisted for the entire observation period in four of the animals (including 1 rabbit with rinsed eye). However the scores were not high enough to classify the test substance as an irritant. Chemosis was also present in all animals with obvious conjunctival swelling persisting for at least 24 hours in 5 of the animals.

The results of this study suggest that ABIL Quat 3270 is not an eye irritant in rabbits.

## **9.2 Overall Assessment of Toxicological Data**

In rat studies, ABIL Quat 3270 had low acute oral toxicity (LD<sub>50</sub> > 5091 mg/kg). It was not an irritant to eyes or skin in the rabbit.

## **10. ASSESSMENT OF ENVIRONMENTAL EFFECTS**

No ecotoxicological data were provided, which is acceptable for polymers of number-average molecular weight greater than 1000 according to the Act.

The high molecular weight of the substance suggests that it will not cross biological membranes, and will therefore be of low toxicity. It is well accepted that polydimethylsiloxane fluids become permanent residents of sediment but should not exert adverse environmental effects. Physical effects such as surface entrapment have been observed when testing aquatic invertebrates in clean laboratory water, but similar effects are not expected in natural environments where a large variety of other surfaces provide opportunities for deposition (1).

While the polymer contains quaternary amine moieties which are known to interact with gill membranes, environmental behaviour of this modified silicone is expected to be dominated by the siloxane backbone, which will rapidly align itself at or on surfaces. The toxicity of quaternary ammonium compounds is known to be greatly reduced in the environment because of preferential

binding to dissolved organics in surface water (9), and the sorptive properties of the polydimethylsiloxane chain will further moderate any toxicity.

## **11. ASSESSMENT OF ENVIRONMENTAL HAZARD**

Polymer waste generated from the formulation of shampoo/conditioner products will be treated at wastewater treatment plants where it is likely to adsorb to sludge. Any polymer that remains in the treated waste water and enters receiving waters is likely to photodegrade to silicates. Therefore, the polymer is unlikely to present a hazard to the aquatic environment.

Disposal of the sludge is unlikely to present a hazard to the environment as incineration would destroy the substance and liberate oxides of carbon, nitrogen and silicon, while disposal to landfill would immobilise it.

Water soluble, polyether substituted polydimethylsiloxane fluids are widely used as home laundry fabric softeners and personal hair care products, applications which involve potential aquatic exposure. The introduction of a similar compound is not expected to lead to a significant increase in environmental hazard, given the biocompatible nature of these substances.

## **12..ASSESSMENT OF PUBLIC AND OCCUPATIONAL HEALTH AND SAFETY EFFECTS**

The notified chemical is a charged polymer with high molecular weight (>1000). It is therefore not likely to cross biological membranes and cause any systemic effects. It contains no toxic impurities, and has been shown in animal studies to have low acute oral toxicity as well as being non-irritant to skin and eyes.

The trade products containing the notified polymer are stable at ambient temperatures, and have no known explosive or reactivity properties, however they contain the hazardous constituent 1,2 propanediol and at high temperatures may form hazardous oxidation products.

Based on the above information, the notified chemical is not expected to pose a significant hazard to occupational health when used in the proposed manner.

As the notified polymer is to be used in commodity products such as shampoos and conditioners, there will be significant public exposure to the notified polymer. Extensive dermal contact is envisaged, and the product type would indicate that the notified polymer may be used repeatedly. As there is no information on the toxicology of the notified polymer following repeated exposure, or on the potential for skin sensitisation, it is considered that the potential public health hazards, following its incorporation into consumer products, have not been adequately studied. The polymer however possesses high molecular weight, and as a result, dermal absorption is anticipated to be low. The likely low systemic exposure is further supported by the pattern of use of the product, where the notified polymer is generally washed a few minutes after application.

### **13. RECOMMENDATIONS**

To minimise occupational exposure (and public/environmental if recommendations have been made by these agencies) to siloxanes and silicones, di Me, 3-[3-[(3-cocoaminopropyl) dimethylammonio] 2-hydroxypropoxy] propyl group terminated, acetates (salts) the following guidelines and precautions should be observed:

- . Suitable personal protective equipment which complies with Australian Standards should be worn during product production, such as chemical-type goggles with face shield recommended to prevent eye contact (10), chemically resistant gloves (11) and protective clothing (12) to prevent skin contact.
- . Good work practices should be implemented to avoid splashing or spillages.
- . Good personal hygiene practices, such as washing of hands prior to eating food, should be observed.
- . A copy of the MSDS for products containing the notified chemical, such as the formulations ABIL Quat 3270 and ABIL Quat 3272, should be easily accessible to employees working with these products.

#### **14. MATERIAL SAFETY DATA SHEET**

The Material Safety Data Sheet (MSDS) for ABIL Quat 3270 and ABIL Quat 3272 (Attachments 1 and 2) were provided in Worksafe Australia format (13). These MSDS were provided by International Sales and Marketing Pty Ltd/Salkat Australia Pty Ltd as part of their notification statement. It is reproduced here as a matter of public record. The accuracy of this information remains the responsibility of International Sales and Marketing Pty Ltd/Salkat Australia Pty Ltd.

#### **15. REQUIREMENTS FOR SECONDARY NOTIFICATION**

Under the *Industrial Chemicals (Notification and Assessment) Act 1989* (the Act), secondary notification of siloxanes and silicones, di Me, 3-[3-[(3-cocoaminopropyl) dimethylammonio] 2-hydroxypropoxy] propyl group terminated, acetates (salts) shall be required if any of the circumstances stipulated under subsection 64(2) of the Act arise. No other specific conditions are prescribed.

#### **16. REFERENCES**

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3. Project No 1-4-566-88 K-3270/50: *Acute oral toxicity in rats*, International Bio Research, 1988.
4. Project No 1-3-568-88 *Test for primary skin irritation of K-3270/50 in rabbits*, International Bio Research, 1988.
5. Project No 1-3-711-88 *Test for eye irritation of K-3270/50 (3%) in rabbits*, International Bio Research, 1988.
6. OECD Guidelines for Testing of Chemicals - *Acute Oral Toxicity* No: 401, 1987.

7. OECD Guidelines for Testing of Chemicals - *Acute Dermal Irritation/Corrosion* No: 404, 1981.
8. OECD Guidelines for Testing of Chemicals - *Acute Eye Irritation/Corrosion* No: 405, 1987.
9. Goodrich M S, Dulak L H, Friedman M A and Lech J J, *Environmental Toxicology and Chemistry*, **10**, 509-515, 1991.
10. Australian Standard 1337-1984 *Eye Protectors for Industrial Applications*, Standards Association of Australia Publ, Sydney, 1984.
11. Australian Standard 2161-1978 *Industrial Safety Gloves and Mittens (excluding Electrical and Medical Gloves)*, Standards Association of Australia Publ, Sydney, 1978.
12. Australian Standard 3765.1-1990 *Clothing for Protection against Hazardous Chemicals Part 1 Protection against General or Specific Chemicals* Standards Association of Australia Publ, Sydney, 1990.
13. National Occupational Health and Safety Commission, *Guidance Note for Completion of a Material Safety Data Sheet*, 3rd Edition, Australian Government Publishing Service Publ., Canberra, 1991.