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# NATIONAL INDUSTRIAL CHEMICALS NOTIFICATION AND ASSESSMENT SCHEME (NICNAS)

## **PUBLIC REPORT**

Poly(oxy-1,4-butanediyl),  $\alpha$ -hydro- $\omega$ -hydroxy-, polymer with 1,3-bis(1-isocyanato-1-methylethyl)benzene and  $\alpha$ -hydro- $\omega$ -hydroxypoly[oxy(methyl-1,2-ethanediyl)], N-[3-(trimethoxysilyl)propyl]carbamate

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

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

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Director NICNAS

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## **SUMMARY**

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

ASSESSMENT REFERENCE	APPLICANT(S)	CHEMICAL OR TRADE NAME	HAZARDOUS CHEMICAL	INTRODUCTION VOLUME	USE
LTD/1885	Henkel Australia Pty	Poly(oxy-1,4-butanediyl), α- hydro-ω-hydroxy-, polymer with	ND*	< 5 tonnes per annum	Component of adhesives
	Ltd	1,3-bis(1-isocyanato-1- methylethyl)benzene and α- hydro-ω- hydroxypoly[oxy(methyl-1,2-			
		ethanediyl)], N-[3- (trimethoxysilyl)propyl]carbamate			

<sup>\*</sup>ND = not determined

## **CONCLUSIONS AND REGULATORY OBLIGATIONS**

#### **Hazard classification**

As no toxicity data were provided, the notified polymer cannot be classified according to the *Globally Harmonised System of 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 in the proposed manner, the notified polymer is not considered to pose an unreasonable risk to public health.

## **Environmental risk assessment**

On the basis of the assessed use pattern, the notified polymer is not considered to pose an unreasonable risk to the environment.

## Recommendations

CONTROL MEASURES

Occupational Health and Safety

• No specific engineering controls, work practices or personal protective equipment are required for the safe use of the notified chemical/polymer itself. However, these should be selected on the basis of all ingredients in the formulation.

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 of Classification and Labelling of Chemicals (GHS)* as adopted for industrial chemicals in Australia, workplace practices and control procedures consistent with provisions of State and Territory hazardous substances legislation should be in operation.

Disposal

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

## Emergency procedures

• Spills or accidental release of the notified polymer should be handled by containment, physical 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 polymer 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 polymer, 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 Da;

or

- (2) Under Section 64(2) of the Act; if
  - the function or use of the polymer has changed from a component of adhesives, or is likely to change significantly;
  - the amount of polymer being introduced has increased, 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)SDSs of the notified polymer and a product containing the notified polymer provided by the notifier were reviewed by NICNAS. The accuracy of the information on the (M)SDSs remains the responsibility of the applicant.

## **ASSESSMENT DETAILS**

## 1. APPLICANT AND NOTIFICATION DETAILS

APPLICANT(S)

Henkel Australia Pty Ltd (ABN: 82 001 302 996)

135-141 Canterbury Road

Kilsyth VIC 3137

NOTIFICATION CATEGORY

Limited: Synthetic polymer with  $Mn \ge 1,000$  Da

EXEMPT INFORMATION (SECTION 75 OF THE ACT)

No details are claimed exempt from publication.

VARIATION OF DATA REQUIREMENTS (SECTION 24 OF THE ACT)

Variation to the schedule of data requirements is claimed for all physico-chemical endpoints

PREVIOUS NOTIFICATION IN AUSTRALIA BY APPLICANT(S)

None

NOTIFICATION IN OTHER COUNTRIES

USA

## 2. IDENTITY OF CHEMICAL

MARKETING NAME(S)

Loctite GO2 gel (containing 66% notified polymer)

CAS NUMBER

716360-25-7

CHEMICAL NAME

Poly(oxy-1,4-butanediyl), α-hydro-ω-hydroxy-, polymer with 1,3-bis(1-isocyanato-1-methylethyl)benzene and α-hydro-ω-hydroxypoly[oxy(methyl-1,2-ethanediyl)], N-[3-(trimethoxysilyl)propyl]carbamate

OTHER NAME(S)

Silane terminated polyurethane

Prepolymer 8606-99

Xtreme Repair

MOLECULAR FORMULA

 $(C_{14}H_{16}N_2O_2.(C_4H_8O)_nH_2O.(C_3H_6O)_nH_2O)_x.xC_7H_{17}NO_5Si$ 

STRUCTURAL FORMULA

MOLECULAR WEIGHT

Number Average Molecular Weight (Mn)5,168 DaWeight Average Molecular Weight (Mw)21,376 DaPolydispersity Index (Mw/Mn)4.1% of Low MW Species < 1,000 Da</td>3.3%% of Low MW Species < 500 Da</td>1.5%

ANALYTICAL DATA

Reference GPC spectra were provided.

## 3. COMPOSITION

DEGREE OF PURITY 99.98%

## HAZARDOUS IMPURITIES/RESIDUAL MONOMERS

Chemical Name Methanol

*CAS No.* 67-56-1 *Weight* % 0.02

Hazardous Properties F; R11

T; R23/24/25 T; R39/23/24/25

Conc. ≥ 20%: T; R23/24/25; R39/23/24/25 10% ≤ Conc. < 20%: T; R20/21/22; R39/23/24/25 3% ≤ Conc. < 10%: Xn; R20/21/22; R68/20/21/22

Non Hazardous Impurities/Residual Monomers (> 1% by Weight) None

## ADDITIVES/ADJUVANTS

Chemical Name Dodecanoic acid, 1,1'-(dibutylstannylene) ester CAS No. 77-58-7 Weight % 0.02

Chemical Name Decanedioic acid, 1,10-bis(2,2,6,6-tetramethyl-4-piperidinyl) ester

CAS No. 52829-07-9 Weight % 1.28

## POLYMER CONSTITUENTS

	CAS No.	Weight %	Weight %
		starting	residual
α-hydro-ω-	25322-69-4	61.77	0
ethyl)-	2778-42-9	6.12	0
droxy-	25190-06-1	26.56	0
thyl-*	406679-89-8	1.73	0
•	15396-00-6	3.83	0
	ethyl)- droxy-	α-hydro-ω- 25322-69-4 ethyl)- 2778-42-9 droxy- 25190-06-1 thyl-* 406679-89-8	starting   α-hydro-ω- 25322-69-4 61.77   ethyl)- 2778-42-9 6.12   droxy- 25190-06-1 26.56   thyl-* 406679-89-8 1.73

<sup>\*</sup>Not included in polymer name as at < 2 wt%

## 4. PHYSICAL AND CHEMICAL PROPERTIES

APPEARANCE AT 20 °C AND 101.3 kPa: clear colourless highly viscous liquid

Property	Value	Data Source/Justification
Melting Point/Freezing Point	Not determined	Liquid at ambient temperature
Boiling Point	Not determined	Expected to be high based on the molecular weight and structure of the notified polymer
Density	$1,000-1,010 \text{ kg/m}^3 \text{ at } 20 ^{\circ}\text{C}$	(M)SDS
Vapour Pressure	Not determined	Expected to be low based on the molecular weight of the notified polymer.
Water Solubility	Not determined	Based on its molecular weight and functional groups the notified polymer is expected to have low water solubility.
Hydrolysis as a Function of pH	Not determined	The notified polymer contains functional groups which are susceptible to hydrolysis, but hydrolysis is expected to

Property	Value	Data Source/Justification
		be slow at environmental pH (4-9). The
		low water solubility of the notified
		polymer is also expected to limit
		hydrolysis.
Partition Coefficient	Not determined	Based on its low water solubility the
(n-octanol/water)		notified polymer is expected to have high
		log Kow.
Adsorption/Desorption	Not determined	Expected to adsorb to soil, sediment and
		sludge due to its expected low water
		solubility and high molecular weight.
Dissociation Constant	Not determined	The notified polymer does not contain
		any functional groups that are expected to
		dissociate in water.
Flash Point	74 °C	Product (M)SDS*
Flammability	Not determined	Not expected to be highly flammable
Autoignition Temperature	Not determined	Not expected to autoignite
Explosive Properties	Not determined	Contains no functional groups that imply
		explosive properties.
Oxidising Properties	Not determined	Contains no functional groups that imply
		oxidative properties.

<sup>\*</sup>For the marketed product Loctite GO2 gel (containing 66% notified polymer)

#### DISCUSSION OF PROPERTIES

## Reactivity

The notified polymer reacts with moisture to release methanol and form a water insoluble polymeric mass.

## Physical hazard classification

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

## 5. INTRODUCTION AND USE INFORMATION

Mode of Introduction of Notified Chemical (100%) Over Next 5 Years

The notified polymer will not be manufactured or reformulated in Australia. The notified polymer will be imported into Australia as a component of finished adhesives at 66% concentration.

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

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

PORT OF ENTRY Melbourne

IDENTITY OF MANUFACTURER/RECIPIENTS

Manufacturer: Henkel (Germany) Recipient: Henkel Australia Pty Ltd

## TRANSPORTATION AND PACKAGING

The notified polymer will be imported as a component of finished adhesives in 18 mL sealed tubes which will be transported to warehousing facilities and then to retail outlets/end-users within Australia by road.

#### USE

Adhesives containing the notified polymer at 66% concentration will be used for binding porous and non-porous substrates such as metal, glass, stone, ceramics, wood and plastics. The adhesives will primarily be used by doit-yourself (DIY) users for small repair jobs. However, the adhesive may also be used by the industrial sector.

#### OPERATION DESCRIPTION

The notified polymer will not be manufactured, reformulated or repackaged in Australia. End users will apply the adhesive containing the notified polymer to substrates directly from the packaging.

#### 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)
Warehouse	< 1	4-10
Transport	1-10	4-10
End-users	1-10	4-10

#### EXPOSURE DETAILS

During transport and storage, workers are unlikely to be exposed to the notified polymer (unless the packaging is accidentally ruptured).

Workers may be exposed to adhesives containing the notified polymer at 66% concentration during removal of the tube seal, transfer of the adhesives from the tube to the substrate and contact with treated substrates before they have cured and dried. Dermal exposure to the notified polymer is expected to be the most likely route of exposure, although accidental ocular and oral exposure is possible. Inhalation exposure to the notified polymer is not expected given the low vapour pressure of the notified polymer and highly viscous nature of the adhesive. In addition, users may have potential for exposure to methanol released from the notified polymer during the curing process. However, given the small size of the tubes, exposure to the notified polymer is expected to be limited. Workers are expected to wear appropriate PPE and use safe work practices to minimise exposure. Once cured and dried following application, the notified polymer will be reacted into the adhesive polymeric matrix and will not be available for exposure.

## **6.1.2.** Public Exposure

DIY users will apply adhesives containing the notified polymer at 66% concentration for small repair jobs. Dermal exposure to the notified polymer is expected to be the most likely route of exposure, although accidental ocular and oral exposure is possible. Inhalation exposure to the notified polymer is not expected given the low vapour pressure of the notified polymer and the highly viscous nature of the adhesive. In addition, users may have potential for exposure to methanol released from the notified polymer during the curing process. However, exposure is expected to be of low frequency and small scale. Once the adhesive is cured, the notified polymer will be incorporated into the matrix and will not be available for exposure.

## 6.2. Human Health Effects Assessment

No toxicity data were submitted.

The notified polymer has a high molecular weight (> 5,000 Da) and a low percentage (3.3%) of low molecular weight species < 1000 Da; hence absorption across biological membranes is expected to be limited. There is a concern for irritation of lungs and mucous membranes based on the reactivity of the notified polymer.

The notified polymer also releases toxic and flammable vapour (methanol) during end-use.

## Health hazard classification

As no toxicity data were provided, the notified polymer cannot be classified according to the *Globally Harmonised System of 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

The main health concern for the notified polymer is the potential for irritation of lungs and mucous membranes from inhalation. Given the expected low vapour pressure of the notified polymer based on its high molecular weight, inhalation exposure is only expected where vapours, mists or aerosols are formed. The notified polymer also releases a toxic and flammable vapour (methanol) during end-use.

## 6.3.1. Occupational Health and Safety

Adhesives containing the notified polymer at 66% concentration will primarily be used by DIY users. However, the adhesive may also be used by the industrial sector. If PPE is used, the exposure of workers is expected to be of a similar or lesser extent than that experienced by DIY users using the adhesives containing the notified polymer. Therefore, the risk to workers from use of the notified polymer is not considered to be unreasonable.

#### 6.3.2. Public Health

Adhesives containing the notified polymer at 66% concentration will be used by DIY users usually for small repairs. Inhalation exposure to the notified polymer is not expected given the viscous nature of the adhesive. DIY users may have potential for inhalation exposure to methanol released from the notified polymer during curing of the adhesive. However, exposure is expected to be of low frequency and small scale. Furthermore, the stated recommended use of adhesive in well-ventilated areas on the product packaging will also limit exposure. Once the adhesive is cured, the notified polymer will be incorporated into the matrix and will not be available for exposure. Therefore when used in the proposed manner, the notified polymer is not considered to pose an unreasonable risk to public health.

## 7. ENVIRONMENTAL IMPLICATIONS

## 7.1. Environmental Exposure & Fate Assessment

## 7.1.1. Environmental Exposure

#### RELEASE OF CHEMICAL AT SITE

The notified polymer or the product containing the notified polymer will not be manufactured or reformulated in Australia. Therefore, no release of the notified polymer to the environment is expected from these activities. In the event of accidental spills and leaks at storage sites, the notified polymer is expected to cure to form a solid mass. The cured solid mass is expected to be collected and disposed of to landfill. Any spills during transportation are not expected to result in significant release to aquatic environments as the notified polymer will form an insoluble solid that can subsequently be collected and disposed of to landfill.

## RELEASE OF CHEMICAL FROM USE

The adhesive containing the notified polymer is designed for the retail market to repair small items. It is expected to be applied to surfaces of both porous and non-porous materials e.g., metal, glass, stone, ceramics, wood and some plastics. A small amount of the notified polymer is expected to be released to the environment due to wastes from spills and during application. Considering the adhesive package size any spills are expected to be small in volume. The notified polymer in these wastes is expected to cure to an inert solid on exposure to ambient conditions and the cured mass will be contained and disposed to landfill or in accordance with relevant state regulations.

## RELEASE OF CHEMICAL FROM DISPOSAL

The majority of the notified polymer will be incorporated in a polymer matrix and bound to the substrate after application. It is expected to share the fate of the substrate and be disposed of to a landfill. Residual product containing the notified polymer is expected to be cured into an inert solid matrix and be disposed of to a landfill along with its packaging.

#### 7.1.2. Environmental Fate

No environmental fate data were submitted for the notified polymer. The majority of the notified polymer is expected to be associated with the substrate surface as part of the adhesive matrix. Since the notified polymer is expected to be cured upon application and become an inert part of the adhesive matrix, it is not expected to be bioavailable to aquatic organisms.

The majority of the notified polymer is expected to be disposed of to landfill with cured articles at the end of their useful life. The notified polymer will eventually degrade biotically or abiotically in landfill to form water and oxides of carbon, nitrogen and silicon.

## 7.1.3. Predicted Environmental Concentration (PEC)

Calculation of the Predicted Environmental Concentration (PEC) is not considered necessary since no significant release of the notified polymer to the aquatic environment is expected from the proposed use pattern.

## 7.2. Environmental Effects Assessment

No ecotoxicity data were submitted. However, no significant release of the notified polymer to the aquatic environment is expected from the proposed use pattern.

## 7.2.1. Predicted No-Effect Concentration

The Predicted No-Effect Concentration (PNEC) has not been calculated since no significant release of the notified polymer to the aquatic environment is expected from the proposed use pattern.

#### 7.3. Environmental Risk Assessment

The risk quotient (Q = PEC/PNEC) for the notified polymer has not been calculated as release to the aquatic environment in ecotoxicologically significant quantities is not expected based on its reported use pattern as a component of an adhesive. The majority of the notified polymer will be disposed of to landfill as a cured polymer matrix. The notified polymer is irreversibly bound in the inert polymer matrix, and is unlikely to be bioavailable or mobile in this form. On the basis of the assessed use pattern and assumed low hazard, the notified polymer is not considered to pose an unreasonable risk to the environment.

## **BIBLIOGRAPHY**

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

United Nations (2009) Globally Harmonised System of Classification and Labelling of Chemicals (GHS), 3rd revised edition. United Nations Economic Commission for Europe (UN/ECE), <a href="http://www.unece.org/trans/danger/publi/ghs/ghs\_rev03/03files\_e.html">http://www.unece.org/trans/danger/publi/ghs/ghs\_rev03/03files\_e.html</a> .