File No: LTD/1438

December 2009

NATIONAL INDUSTRIAL CHEMICALS NOTIFICATION AND ASSESSMENT SCHEME (NICNAS)

FULL PUBLIC REPORT

1-Propanamine, N,N-dimethyl-3-(octadecyloxy)-
[INCI Name: Stearoxypropyl dimethylamine]

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, Water, Heritage and the Arts.

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:

Street Address:	334 - 336 Illawarra Road MARRICKVILLE NSW 2204, AUSTRALIA.
Postal Address:	GPO Box 58, SYDNEY NSW 2001, AUSTRALIA.
TEL:	+ 61 2 8577 8800
FAX	+ 61 2 8577 8888
Website:	www.nicnas.gov.au

Director
NICNAS

TABLE OF CONTENTS

FULL PUBLIC REPORT

1-Propanamine, N,N-dimethyl-3-(octadecyloxy)-
[INCI Name: Stearoxypropyl dimethylamine]

1. APPLICANT AND NOTIFICATION DETAILS

APPLICANT(S)
Kao Brands Australia Pty Ltd (ABN 72 111 285 146)
Level 1, 19 Prospect Street
BOX HILL VIC 3128

NOTIFICATION CATEGORY
Limited-small volume: Chemical other than polymer (1 tonne or less per year).

EXEMPT INFORMATION (SECTION 75 OF THE ACT)
Data items and details claimed exempt from publication: Spectral Data, Degree of Purity, Use Details.

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

NOTIFICATION IN OTHER COUNTRIES
Canada

2. IDENTITY OF CHEMICAL

CHEMICAL NAME
1-Propanamine, N,N-dimethyl-3-(octadecyloxy)-

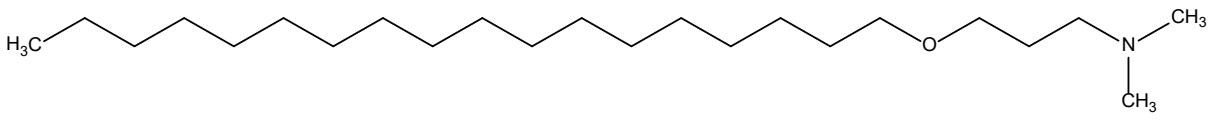
OTHER NAME(S)
Stearoxypropyl dimethylamine (INCI Name)
Propylamine, N,N-dimethyl-3-(octadecyloxy)-
Farmin DM E80
Stearoxypropyldimethylamine

MARKETING NAME(S)
FR-80
Sheer Blonde Highlight Activating Enhancing Conditioner (containing < 0.5% notified chemical)

CAS NUMBER
17517-01-0

MOLECULAR FORMULA
$C_{23}H_{49}NO$

STRUCTURAL FORMULA



MOLECULAR WEIGHT
355.64 Da.

ANALYTICAL DATA
Reference ^{1}H NMR, IR, and UV spectra were provided.

3. COMPOSITION

DEGREE OF PURITY
> 80%

4. PHYSICAL AND CHEMICAL PROPERTIES

APPEARANCE AT 20°C AND 101.3 kPa: White, waxy solid

Property	Value	Data Source/Justification
Melting/Pour Point	27°C	Measured
Boiling Point	390 °C at 101.55 kPa	Measured
Density	880 kg/m^3 at 20°C	Measured
Vapour Pressure	1.8x10^{-8} kPa at 25°C	Measured
Water Solubility	< 5×10^{-5} g/L at 20.0±0.5°C	Measured
Hydrolysis as a Function of pH	Not determined	The notified chemical does not contain functionality that is expected to hydrolyse within the environmental pH range of 4-9.
Partition Coefficient (n-octanol/water)	log P_{ow} > 6.50 at 20°C	Measured for the neutral form.
Adsorption/Desorption	Not determined	The notified chemical will act as a cationic surfactant within the environmental pH range of 4-9, and is expected to appreciably adsorb to soil and sediment.
Dissociation Constant	pK_a = 8.2	Measured in 20% water in ethanol by an unspecified method.
Particle Size	Not determined	Imported in finished product. Notified chemical melts at temperatures slightly above room temperature.
Flammability	Not determined	Not expected to be flammable in imported mixture
Autoignition Temperature	Not determined	Not expected to autoignite under normal conditions of use
Flash Point	> 187°C	For the notified chemical as stated by the notifier (Test data not available)
	> 61 °C	MSDS for product containing the notified chemical
Explosive Properties	Not determined	Does not contain explosophores

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

Reactivity
The notified chemical is expected to be stable under normal environmental conditions.

5. INTRODUCTION AND USE INFORMATION

MODE OF INTRODUCTION OF NOTIFIED CHEMICAL (100%) OVER NEXT 5 YEARS
The notified chemical will be imported at concentrations of < 0.5% in the finished hair conditioner product Sheer Blonde Highlight Activating Enhancing Conditioner.

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

TRANSPORTATION AND PACKAGING
The notified chemical will be imported by sea as a component (< 0.5%) of finished hair conditioner products in 250 mL plastic bottles. Boxes containing 6 bottles of hair conditioner will be transported to the notifier in Victoria for distribution to retail outlets by road.

USE
The notified chemical will be used as a surfactant at < 0.5% concentration in hair conditioner products.

OPERATION DESCRIPTION
The notified chemical will not be reformulated or repackaged in Australia. Finished hair conditioner products containing the notified chemical will be used by consumers and in professional settings by hair salon workers. Hairdressers will apply the conditioner product directly to the wet hair of customers, leave for several minutes and then rinse off.

6. HUMAN HEALTH IMPLICATIONS

6.1 Exposure assessment

6.1.1 Occupational exposure

NUMBER AND CATEGORY OF WORKERS

Category of Worker	*Number*	*Exposure Duration (hours/day)*	*Exposure Frequency (days/year)*
Transport and storage	10	4	365
Recycling and disposal	5	2	365
Hair salon workers	> 1000	1-2	Variable

EXPOSURE DETAILS
Exposure to the hair conditioner containing the notified chemical at < 0.5% is not anticipated during transport and distribution to retail outlets.

Occupational exposure is expected for workers in hair and beauty salons using products containing the notified chemical (< 0.5%). Dermal exposure is expected to be extensive given that hair conditioner products containing the notified chemical will be applied using the hands and that gloves are unlikely to be worn. Accidental ocular exposure and oral ingestion may also occur.

The level of dermal exposure to workers is likely to be greater than that expected for the public (see below).

6.1.2. Public exposure
Public exposure to the notified chemical is expected to be widespread and frequent through regular use of hair conditioner products containing the notified chemical at concentrations up to 0.5%. Exposure to the notified chemical will vary depending on individual use patterns. The principal route of exposure will be dermal, while accidental ocular exposure is also possible. Accidental ingestion from the use of these types of products is also possible though is not expected to be significant during normal use.

Systemic exposure to the notified chemical is estimated below using the EU Scientific Committee on Consumer Products' (SCCP's) default values for rinse-off conditioner products and applying the following assumptions:

- Bodyweight of 60 kg (SCCP, 2006);
- The concentration of the notified chemical in hair conditioner products is 0.5%;
- 100% dermal absorption (in the absence of absorption data);

Product	*Exposure level*	*Retention factor*	*Systemic Exposure* (mg/kg bw/day)*
Conditioner	14.00 g x 0.28 applications/day x 0.5% concentration	0.01	0.003

* Systemic exposure = Exposure x retention factor/Bodyweight

6.2. Human health effects assessment

The results from toxicological investigations conducted on the notified chemical are summarised in the table below.

Endpoint	*Result and Assessment Conclusion*
Rat, acute oral toxicity	oral LD50 > 2000 mg/kg bw low toxicity
Mutagenicity – bacterial reverse mutation	non mutagenic

Toxicokinetics
Limited data is available to describe the likely toxicokinetic properties of the notified chemical. It has low molecular weight (< 500 Da.), low water solubility (< 1 mg/L) and high lipophilicity (log P_{ow} > 6.5) which suggests that absorption across the skin may occur to a small degree. This may be enhanced by its surfactant properties and expected skin irritancy based on the presence of a functional group with a structural alert for corrosion/irritation. Absorption across the gastrointestinal tract may occur by micellular solubilisation, given its highly lipophilic nature and low water solubility.

Acute toxicity
The notified chemical was tested in an acute oral toxicity study in female rats at 300 and 2000 mg/kg bw conducted according to OECD TG 420 (Safepharm Laboratories Ltd, 2007c). The notified chemical was administered as a solution in arachis oil BP by oral gavage. No mortality was observed at either dose level. No signs of systemic toxicity were observed in the animals treated with 300 mg/kg bw. The following clinical observations were reported in four of the five animals treated with 2000 mg/kg bw: hunched posture, diarrhoea, pilo-erection, diuresis, and red/brown staining around the ano-genital region and eyes. These observations persisted for either 4, 5 or 6 days after dosing. Overall, the notified chemical was found to be of low acute toxicity (LD_{50} > 2000 mg/kg bw) following oral exposure.

No data was available on the acute toxicity following dermal or inhalation exposure. Given the relatively low dermal absorption expected the acute dermal toxicity is expected to be low.

Irritation and Sensitisation
Skin and eye irritation tests on the notified chemical were not provided. The notified chemical contains a tertiary amine group that is a structural alert for corrosion/irritation. Two structurally related chemicals ((N,N-Dimethyldodecylamine (CAS No. 112-18-5) and Amines, C12-14-alkyldimethyl- (CAS No. 84649-84-3) are also known to be irritating or corrosive to the skin and eyes (OECD, 2001, ICSC-IPCS (2004)). The notified chemical shares a tertiary amine functionality with the two structurally related chemicals but it also contains an ether functionality and a much longer alkyl chain. Despite these differences with the structurally related chemicals, the notified chemical is still expected to cause significant skin and eye irritation.

No information on the skin sensitisation potential of the notified chemical or structurally related chemicals was available.

Repeated Dose Toxicity
A repeated dose toxicity test on the notified chemical was not provided. A report on a 28-day subchronic toxicity study conducted according to OECD TG407 on N,N-Dimethyldodecylamine (CAS No. 112-18-5) (OECD (2001)) at dose levels of 50, 150 and 300 mg/kg bw/day reported deaths in 3/5 females dosed at 300 mg/kg bw/day with no deaths reported at lower doses. A No Observed Effect Level (NOEL) of 50 mg/kg bw/day was established. The notified chemical may have lower toxicity than this related chemical as it is likely to have lower dermal absorption due to its higher molecular weight.

Mutagenicity
The notified chemical (dissolved in acetone) failed to induce an increase in revertant colonies at concentrations up to 5000 µg/plate in a bacterial reverse mutation assay (Ames test), conducted both with and without metabolic activation according to the method described in OECD TG 471 (Safepharm 2007d). Evidence of reduction of the

background lawn was reported at ≥ 150 µg/plate in the *Salmonella* strains (TA1535, TA1537, TA98 an TA100) with or without metabolic activation but not in the *E. coli* strain (wP2uvrA$^-$). Precipitate was observed at doses ≥ 500 µg/plate but this did not prevent scoring. There were no increases in the frequency of revertant colonies for any of the bacterial strains at any dose levels in the presence or absence of metabolic activation.

Toxicity for reproduction

A reproduction/developmental toxicity study on a structurally related chemical N,N-Dimethyldodecylamine (CAS No. 112-18-5) (OECD (2001)) showed several mortalities. The NOEL for both parent animals and pups was established as 50 mg/kg bw/day.

Health hazard classification

Based on the reported irritation/corrosive effects of structurally related chemicals ((N,N-Dimethyldodecylamine (CAS No. 112-18-5) and Amines, C12-14-alkyldimethyl- (CAS No. 84649-84-3)) and due to the presence of a tertiary amine group in the notified chemical it should be considered as hazardous, with the following risk phrase: irritating to eyes and skin (R36/38).

6.3. Human health risk characterisation

6.3.1. Occupational health and safety

The notified chemical is considered to be a skin and eye irritant based on the results of studies on structurally related chemicals.

The main route of exposure for workers in hair and beauty salons using hair conditioner products containing the notified chemical (≤ 0.5%) is expected to be dermal. However, exposure to the notified chemical at this concentration is not expected to lead to skin irritation.

A NOAEL was not determined for the notified chemical itself but repeated exposure experienced by workers in health and beauty salons is not anticipated to result in adverse effects due to the very low concentration of the notified chemical in hair conditioner products.

Overall, the notified chemical is not considered to pose an unacceptable risk to workers in hair and beauty salons at the concentration used in hair conditioner products (≤ 0.5%).

6.3.2. Public health

Members of the public may be repeatedly exposed via the dermal and perhaps ocular routes during use of hair conditioner products containing the notified chemical at concentrations ≤ 0.5%. The risk of skin or eye irritancy effects is not considered to be unacceptable, given the very low concentrations of the notified chemical in products.

Overall, the risk to public health presented by the notified chemical present at ≤ 0.5% in hair conditioner products is not considered to be unacceptable.

7. ENVIRONMENTAL IMPLICATIONS

7.1. Environmental Exposure & Fate Assessment

7.1.1 Environmental Exposure

RELEASE OF CHEMICAL AT SITE

The notified chemical will be imported into Australia as a component of a finished hair conditioner product for direct end-use in Australia. No local reformulation or repackaging will take place and therefore no significant release is expected to occur in Australia as a result of these processes.

RELEASE OF CHEMICAL FROM USE

The notified chemical is a component of a hair conditioner, which will be directly applied to the consumer's hair. The hair conditioner will then be rinsed off and go down the sink/drain, and enter the drainage/sewerage system where it will be taken to various waste water treatment facilities.

RELEASE OF CHEMICAL FROM DISPOSAL

The hair conditioner bottles, containing the notified chemical, should 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 minimal amounts of residual notified chemical within the bottles.

7.1.2 Environmental fate

Two fate studies were provided for the notified chemical. The results of a ready biodegradability study showed that the notified chemical cannot be classified as being ready biodegradable. However, the results of an inherent degradability study showed that the notified chemical is inherently degradable. For the details of the environmental fate studies please refer to Appendix C.

It is anticipated that almost all of the imported product containing the notified chemical will go to the sewerage system via rinsing after hair application. The SimpleTreat Model (European Commission, 2003) estimates that up to 87% of the quantity of notified chemical being disposed to sewer may be removed in the sewage treatment plant. Another study (Games *et al.*, 1982) indicates that more than 99% of quaternary ammonium surfactants may be removed in a sewage treatment plant via both absorption to solids and biodegradation. Based on this, it is anticipated that only very low concentrations of the notified chemical will be discharged to surface waters from sewage treatment plants. As the notified chemical is a cationic surfactant it is expected to adsorb to surfaces in the environment, rather than remain dissolved in the water column. Although the notified chemical has a high log K_{ow}, it is a cationic surfactant and is therefore unlikely to bioaccumulate.

7.1.3 Predicted Environmental Concentration (PEC)

Assuming that most of the notified chemical will be washed into the sewer, the following Predicted Environmental Concentration (PEC) in sewage effluent on a nationwide basis was calculated allowing for 87% mitigation (4% degradation and 83% partitioning to sludge), leaving 13% of the annual introduction volume remaining in effluent, as estimated by the SimpleTreat Model (European Commission, 2003).

Predicted Environmental Concentration (PEC) for the Aquatic Compartment		
Total Annual Import 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	21.161	million
Removal within STP	87%	**Mitigation**
Daily effluent production:	4,232	ML
Dilution Factor - River	1.0	
Dilution Factor - Ocean	10.0	
PEC - River:	0.084	µg/L
PEC - Ocean:	0.008	µg/L

7.2. Environmental effects assessment

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

Endpoint	*Result*	*Assessment Conclusion*
Fish Toxicity[*]	96 h LC50 0.13 mg/L	Very toxic to fish
Daphnia Toxicity[**]	48 h EC50 0.18 mg/L	Very toxic to aquatic invertebrates
Algal Toxicity	72 h E_rC50 0.026 mg/L[***]	Very toxic to algae

[*] Result for analogue chemical (Hydrochloride salt of the notified chemical)
[**] Result for analogue chemical (SP-01-02)
[***] Based on the geometric mean exposure concentrations

7.2.1 Predicted No-Effect Concentration

Using the most sensitive endpoint, and an assessment factor of 100, the Predicted No-Effect Concentration for the aquatic compartment has been determined as follows:

Predicted No-Effect Concentration (PNEC) for the Aquatic Compartment		
EC50 (Alga)	0.026	mg/L
Assessment Factor	100	
PNEC:	0.260	µg/L

7.3. Environmental risk assessment

Based on the above calculations the Risk Quotient (PEC/PNEC) has been calculated as follows:

Risk Assessment	*PEC µg/L*	*PNEC µg/L*	*Q*
Q - River:	0.084	0.260	0.324
Q - Ocean:	0.008	0.260	0.032

Based on the above calculation for Risk Quotient, the notified chemical is not expected to pose an unacceptable risk to the environment from the proposed use of the hair conditioner product containing the notified chemical at the maximum importation volume. However, the risk quotient for discharge of treated effluents containing the notified chemical to riverine environments is relatively narrow as a result of the high acute toxicity of this chemical.

Partitioning to biosolids in STPs Australia-wide may result in an average biosolids concentration of 5.373 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 1500 kg/m^3 and a soil-mixing zone of 10 cm, the concentration of the notified chemical may approximate 0.036 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 0.18 mg/kg and 0.36 mg/kg, respectively. This latter scenario is unlikely as the notified chemical is inherently biodegradable.

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 10 cm of soil (density 1500 kg/m^3). Using these assumptions, irrigation with a concentration of 0.084 µg/L may potentially result in a soil concentration of approximately 5.610×10^{-4} 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 2.805×10^{-3} mg/kg and 5.610×10^{-3} mg/kg, respectively. The notified chemical is unlikely to be mobile in soil environments based on its expected affinity for soil. This property, together with its inherent biodegradability indicate a limited potential to leach through the soil horizon.

8. CONCLUSIONS AND REGULATORY OBLIGATIONS

Hazard classification

Due to the limited information provided, the notified chemical cannot be classified using the *Approved Criteria for Classifying Hazardous Substances* (NOHSC, 2004). However, based on the reported irritation/corrosive effects of structurally related chemicals (N,N-Dimethyldodecylamine (CAS No. 112-18-5) and Amines, C12-14-alkyldimethyl- (CAS No. 84649-84-3)) and due to the presence of a tertiary amine group in the notified chemical, it should be considered as hazardous with the following risk phrase:

R36/38 Irritating to eyes and skin.

As a comparison only, the classification of the notified chemical using the Globally Harmonised System for the Classification and Labelling of Chemicals (GHS) (United Nations 2009) 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*

Health	Skin - Category 2	Causes skin irritation
	Eye - Category 2	Causes eye irritation
Environment	Acute I	Very toxic to aquatic life
	Chronic I	Very toxic to aquatic life with long lasting effects

The notified chemical is classified as an "environmentally hazardous substance (aquatic environment)" under the *Australian Dangerous Goods Code 7th edition* (NTC, 2007).

Human health risk assessment
Under the conditions of the occupational settings described, the notified chemical is not considered to pose an unacceptable risk to the health of workers.

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

Environmental risk assessment
On the basis of the PEC/PNEC ratio, reported use pattern, and proposed annual introduction volume, the notified chemical is not expected to pose a risk to the environment.

Recommendations

REGULATORY CONTROLS
Hazard Classification and Labelling

- Based on the reported irritation/corrosive effects of structurally related chemicals (N,N-Dimethyldodecylamine (CAS No. 112-18-5) and Amines, C12-14-alkyldimethyl- (CAS No. 84649-84-3)) and due to the presence of a tertiary amine group in the notified chemical, it should be considered as hazardous with the following risk phrase:

  R36/38 Irritating to eyes and skin.

- The notified chemical is classified as an "environmentally hazardous substance (aquatic environment)" under the *Australian Dangerous Goods Code 7th edition* (NTC, 2007).

CONTROL MEASURES
Occupational Health and Safety

- 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.

Regulatory Obligations

Secondary Notification
This risk assessment is based on the information available at the time of notification. The Director may call for the reassessment of the chemical under secondary notification provisions based on changes in certain circumstances. Under Section 64 of the *Industrial Chemicals (Notification and Assessment) Act (1989)* the notifier, as well as any other importer or manufacturer of the notified chemical, have post-assessment regulatory obligations to notify NICNAS when any of these circumstances change. These obligations apply even when the notified chemical is listed on the Australian Inventory of Chemical Substances (AICS).

Therefore, the Director of NICNAS must be notified in writing within 28 days by the notifier, other importer or manufacturer:

(1) Under Section 64(1) of the Act; if
- the importation volume exceeds one tonne per annum notified chemical;
- the concentration of the notified chemical in hair conditioners exceeds 0.5%;

or

(2) Under Section 64(2) of the Act; if
- the function or use of the chemical has changed from a component of hair conditioner products;
- the chemical has begun to be manufactured in Australia;
- additional information has become available to the person as to an adverse effect of the chemical on occupational health and safety, public health, or the environment.

The Director will then decide whether a reassessment (i.e. a secondary notification and assessment) is required.

Material Safety Data Sheet
The MSDS of a product containing the notified chemical 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/Pour Point 27 ± 3°C

Method	OECD TG 102 Melting Point/Melting Range.
Remarks	Pour point measurement.
Test Facility	Safepharm (2007a)

Boiling Point 390 ± 1°C at 101.55 kPa

Method	OECD TG 103 Boiling Point.
Test Facility	Safepharm (2007a)

Density 880 kg/m^3 at 20 ± 0.5°C

Method	OECD TG 109 Density of Liquids and Solids.
Remarks	Pycnometer method
Test Facility	Safepharm (2007a)

Vapour Pressure $1.8x10^{-8}$ kPa at 25°C

Method	OECD TG 104 Vapour Pressure.
Remarks	Vapour pressure balance
Test Facility	Safepharm (2007b)

Water Solubility < 5×10^{-5} g/L at 20.0 ± 0.5°C

Method	OECD TG 105 Water Solubility
Remarks	Flask Method (determined at pH 7.2 to 7.6.) used as Column Elution Method was unable to be used due to the physical nature of the test substance. Soft, waxy test material coated onto glass beads caused these beads to compact and adhere together, forming a plug within the column and thus prevented water circulation. The notified chemical formed stable emulsions under the test conditions that needed to be filtered prior to analysis by HPLC. The notified chemical is surface active and the ionic form of this amphoteric substance is expected to be more soluble in water.
Test Facility	Safepharm (2007)

Partition Coefficient (n-octanol/water) log P_{ow} > 6.50 at 20°C

Method	OECD TG 117 Partition Coefficient (n-octanol/water)
Remarks	HPLC Method at pH 12. The notified chemical eluted after the reference substance DDT (with 100% methanol). The partition coefficient of the ionised form of the test material at pH 7 was estimated to be log P_{ow} = 6.18 using KOWWIN and a calculated value for the pK_a (9.42 ACD, pK_a).
Test Facility	Safepharm (2007)

Dissociation Constant pK_a = 8.2 (close analogue)

Method	Not specified
Remarks	The pK_a of the close analogue of the notified chemical was reported as 8.2 in a 2:8 mixture of water and ethanol.
Test Facility	Japan Clinical Laboratories, Inc. (2001)

APPENDIX C: ENVIRONMENTAL FATE AND ECOTOXICOLOGICAL INVESTIGATIONS

C.1. Environmental Fate

C.1.1. Ready biodegradability

TEST SUBSTANCE Notified chemical

METHOD OECD TG 301 B Ready Biodegradability: CO_2 Evolution Test.
Inoculum Activated Sewage Sludge
Exposure Period 29 days
Auxiliary Solvent Nil
Analytical Monitoring DOC
Remarks - Method No significant protocol deviations were reported.

RESULTS

Test substance		*Sodium benzoate*	
Day	*% Degradation*	*Day*	*% Degradation*
2	0	2	14
6	1	6	38
10	18	10	64
16	27	16	66
22	20	22	93
27	18	27	75
28	21	28	90
29*	22	29	90

*Day 29 values corrected to include any carry-over of CO_2 detected in Absorber 2.

Remarks - Results All test validity criteria were satisfied.

CONCLUSION The notified chemical is not readily biodegradable

TEST FACILITY Safepharm (2007e)

C.1.2. Inherent degradability

TEST SUBSTANCE Notified chemical

METHOD OECD TG 302C Inherent Biodegradability: Modified MITI Test (II).
Inoculum Standard Activated Sludge
Exposure Period 28 days
Auxiliary Solvent n-hexane/chloroform (7:3 v/v)
Analytical Monitoring BOD, TOC, GC
Remarks – Method No significant protocol deviations were reported.

RESULTS

Test substance		*Aniline*	
Day	*% Degradation*	*Day*	*% Degradation*
28 – BOD	69.2	7	60.4
28 – TOC	98.6	14	66.3
28 – GC	100.0		

Remarks – Results All test validity criteria were satisfied.

CONCLUSION The notified chemical is inherently degradable.

TEST FACILITY Japan Clinical Laboratories, Inc. (2001)

C.2. Ecotoxicological Investigations

C.2.1. Acute toxicity to fish

TEST SUBSTANCE	Hydrochloride salt of notified chemical
METHOD	OECD TG 203 Fish, Acute Toxicity Test - Static
Species	Rainbow Trout (*Oncorhynchus mykiss*)
Exposure Period	96 hours
Auxiliary Solvent	Nil
Water Hardness	100 mg $CaCO_3$/L
Analytical Monitoring	None reported
Remarks – Method	No deviations from the protocol used. Precipitation of test material was observed at 100 mg/L test concentration in range finding study. The toxicity endpoints were calculated based on nominal concentrations.

RESULTS

Concentration mg/L		*Number of Fish*	*Mortality*				
Nominal	*Actual*		*6 h*	*24 h*	*48 h*	*72 h*	*96 h*
0		10	0	0	0	0	0
0.1		10	0	0	0	0	0
0.18		10	0	0	10	10	10
0.32		10	0	6	10	10	10
0.56		10	0	10	10	10	10
1.0		10	2	10	10	10	10

LC50	0.13 mg/L at 96 hours (95% C.I. = 0.10 – 0.18 mg/L)
NOEC	0.10 mg/L at 96 hours
Remarks – Results	Effects of exposure (other than death) were swimming at the surface and loss of equilibrium.
CONCLUSION	The analogue chemical is very toxic to fish
TEST FACILITY	Safepharm (1995)

C.2.2. Acute toxicity to aquatic invertebrates

TEST SUBSTANCE	SP-01-02
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	250 mg $CaCO_3$/L
Analytical Monitoring	Nil at request of sponsor
Remarks - Method	No significant protocol deviations were reported. Observation of the test media showed all test solutions to be clear throughout the study.

RESULTS

Concentration mg/L		*Number of D. magna*	*Number Immobilised*	
Nominal	*Actual*		*24 h*	*48 h*
0		20	0	0
0.10		20	0	0

0.18	20	0	9
0.32	20	0	20
0.56	20	5	20
1.0	20	20	20
1.8	20	20	20
3.2	20	20	20
5.6	20	20	20
10	20	20	20

EC50	0.18 mg/L at 48 hours (95% C.I. = 0.16 – 0.21 mg/L)
NOEC	0.10 mg/L at 48 hours
Remarks - Results	All test validity criteria were satisfied.

CONCLUSION The analogue chemical is very toxic to aquatic invertebrates

TEST FACILITY Safepharm (2002)

C.2.3. Algal growth inhibition test

TEST SUBSTANCE Notified chemical

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, 0.00625, 0.0125, 0.025, 0.050 and 0.10 mg/L Geometric mean measured over 72 hours: 0, 0.00081, 0.0011, 0.0016, 0.022 and 0.035 mg/L
Auxiliary Solvent	Nil
Analytical Monitoring	HPLC
Remarks - Method	Reference substance = Potassium dichromate. No significant protocol deviations were reported.

RESULTS

Biomass		*Yield*		*Growth*	
E_bC_{50} *mg/L at 0-72 h*	NOE_bC *mg/L*	E_yC_{50} *mg/L at 0-72 h*	NOE_yC *mg/L*	E_rC_{50} *mg/L at 0-72 h*	NOE_rC *mg/L*
0.017	0.0016	0.0071	0.0016	0.026	0.0016
95% C.I.		95% C.I.		95% C.I.	
0.015 – 0.019		0.0050 – 0.010		0.024 – 0.027	

Remarks - Results Analysis of the test preparation at 0 hours showed measured test concentrations to range from 87 – 94% of nominal. A decline in measured concentration was observed at 72 hours in the range of less than the limit of quantitation (LOQ) of the analytical method employed which was assessed down to 0.00023 mg/L to 20% of nominal. The decline was considered to be due to a combination of both the slightly light unstable nature of the test material as was seen in the preliminary stability analyses conducted and adsorption to the algal cells present. Given this decline in measured test concentrations it was considered justifiable to base the results on the geometric mean measured test concentrations in order to give a "worst case" analysis of the data. A well defined dose-response curve was obtained over the concentration range tested.

All test validity criteria were satisfied.

CONCLUSION The notified chemical is very toxic to algae.

TEST FACILITY Safepharm (2008)

BIBLIOGRAPHY

European Commission (2003). Technical Guidance Document on Risk Assessment in Support of Commission Directive 93/67/EEC on Risk Assessment for New Notified Substances and Commission Regulation (EC) No 1488/94 on Risk Assessment for Existing Substances and Directive 98/8/EC of the European Parliament and of the Council Concerning the Placing of Biocidal Products on the Market – Part II. Institute for Health and Consumer protection, European Chemicals Bureau, European Communities.

Games, LM & King JE (1982) Fate and Distribution of a Quaternary Ammonium Surfactant, Octadecyltrimethylammonium Chloride (OTAC), In Wastewater Treatment, Environ. Sci. Technol. **16**: 483-488.

IUCLID (2004) Amines, C12-14-alkyldimethyl (CAS No. 84649-84-3) (EC No. 283-464-9) IUCLID Dataset, UNEP Publications. Available online [29 September 2009]: http://www.oecd.org/document/55/0,2340,en_2649_34379_31743223_1_1_1_1,00.html

Japan Clinical Laboratories, Inc. (2001) Inherent Degradability Study of FARMIN DM E-80 by Microbes etc. Report No. JCL018142. Nishiwaki Laboratory, Bioassay Division, Japan Clinical Laboratories, Inc. Nishiwaki City, Hyogo Prefecture, Japan. 12 December 2001 (Unpublished report provided by notifier)

NOHSC (1994) National Code of Practice for the Labelling of Workplace Substances [NOHSC:2012(1994)]. National Occupational Health and Safety Commission, Canberra, Australian Government Publishing Service.

NOHSC (2003) National Code of Practice for the Preparation of Material Safety Data Sheets, 2nd edition [NOHSC:2011(2003)]. National Occupational Health and Safety Commission, Canberra, Australian Government Publishing Service.

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

NTC (National Transport Commission) 2007 Australian Code for the Transport of Dangerous Goods by Road and Rail (ADG code), 7th Edition, Commonwealth of Australia

OECD (2001) SIDS Initial Assessment Report for SIAM 11. N,N-Dimethyldodecylamine (CAS No. 112-18-5). OECD SIDS, UNEP Publications. Available online [29 September 2009]: http://www.inchem.org/documents/sids/sids/112185.pdf.

Safepharm Laboratories Ltd (1995) Acute Toxicity to Rainbow Trout. Project No. 140/338. Safepharm Laboratories Ltd, Derby, United Kingdom. 7 August 1995 (Unpublished report provided by notifier)

Safepharm Laboratories Ltd (2002) Acute Toxicity to *Daphnia Magna*. Project No. 140/1071. Safepharm Laboratories Ltd, Derby, United Kingdom. 3 January 2002 (Unpublished report provided by notifier)

Safepharm Laboratories Ltd (2007a) Determination of General Physico-Chemical Properties. Project No. 0140/1418. Safepharm Laboratories Ltd, Derbyshire, United Kingdom. 20 September 2007 (Unpublished report provided by notifier)

Safepharm Laboratories Ltd (2007b) Determination of Vapour Pressure. Project No. 0140/1419. Safepharm Laboratories Ltd, Derbyshire, United Kingdom. 7 September 2007 (Unpublished report provided by notifier)

Safepharm Laboratories Ltd (2007c) Acute Oral Toxicity in the Rat – Fixed Dose Method. Project No. 0140/1420. Safepharm Laboratories Ltd, Derbyshire, United Kingdom. 26 September 2007 (Unpublished report provided by notifier)

Safepharm Laboratories Ltd (2007d) Reverse Mutation Assay "AMES Test" using *Salmonella Typhimurium* and *Escherichia Coli*. Project No. 0140/1421. Safepharm Laboratories Ltd, Derbyshire, United Kingdom. 26 September 2007 (Unpublished report provided by notifier)

Safepharm Laboratories Ltd (2007e) Assessment of Ready Biodegradability; CO_2 Evolution Test. Project No. 0140/1430. Safepharm Laboratories Ltd, Derbyshire, United Kingdom. 31 October 2007 (Unpublished report provided by notifier)

Safepharm Laboratories Ltd (2008) Algal Growth Inhibition Test. Project No. 0140/1422. Safepharm Laboratories Ltd, Derbyshire, United Kingdom. 8 February 2008 (Unpublished report provided by notifier)

United Nations (2003) Globally Harmonised System of Classification and Labelling of Chemicals (GHS). United Nations Economic Commission for Europe (UN/ECE), New York and Geneva.