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NATIONAL INDUSTRIAL CHEMICALS NOTIFICATION AND ASSESSMENT SCHEME

FULL PUBLIC REPORT

DODECANOIC ACID, DIMETHYLOCTYL ESTER

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Director
Chemicals Notification and Assessment

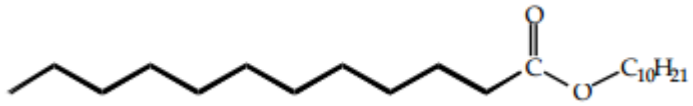
FULL PUBLIC REPORT

Dodecanoic acid, dimethyloctyl ester

1. APPLICANT

Johnson & Johnson Pacific Pty Ltd of Stephen Road BOTANY NSW 2019 has submitted a limited notification statement in support of their application for an assessment certificate for dodecanoic acid, dimethyloctyl ester.

2. IDENTITY OF THE CHEMICAL

Chemical Name:	dodecanoic acid, dimethyloctyl ester
Chemical Abstracts Service (CAS) Registry No.:	94247-10-6
Other Names:	isodecyl laurate isodecyl dodecanoate
Marketing Name:	Isostearene
Molecular Formula:	$C_{22}H_{44}O_2$
Structural Formula:	
Molecular Weight:	340.57
Method of Detection and Determination:	infrared spectroscopy (IR)
Spectral Data:	characteristic peaks were found in the IR spectrum at: 1 115, 1 175, 1 245, 1 380, 1 470, 1 740, 2 825 and 2 901 cm^{-1}

3. PHYSICAL AND CHEMICAL PROPERTIES

Appearance at 20°C and 101.3 kPa:	colourless or pale yellow liquid
Boiling Point:	not determined (see comments below)
Specific Gravity:	0.862 ±1% at 20°C
Vapour Pressure:	not determined (see comments below)
Water Solubility:	not determined (see comments below)
Partition Co-efficient (n-octanol/water):	see comments (below)
Hydrolysis as a Function of pH:	not determined (see comments below)
Adsorption/Desorption:	not determined (see comments below)
Dissociation Constant:	not determined (see comments below)
Flash Point:	238°C
Flammability Limits:	not determined
Autoignition Temperature:	not determined
Explosive Properties:	not determined
Reactivity/Stability:	stable under room conditions

Comments on Physico-Chemical Properties

The physico-chemical data presented in the notification dossier were extremely limited.
The boiling point of the chemical was not supplied. *Environment Australia* estimates the boiling point to be 397°C based on quantitative structure activity relationship (QSAR) calculation using the US EPA ASTER program (1).

The vapour pressure of the chemical has not been determined. Estimation of the vapour pressure for the chemical using QSAR calculations gave a value of 8.33×10^{-9} mm Hg (1), indicating that the chemical is not expected to volatilise.

The water solubility of the chemical has not been determined. A water solubility for the chemical of 6.16×10^{-6} mg/L was estimated using QSAR calculations (1), indicating that the

chemical is expected to have a very low solubility in water.

The hydrolytic decomposition of the chemical has not been investigated. The chemical contains an ester link which could potentially undergo hydrolysis. However, the expected low water solubility of the chemical would indicate that any hydrolysis would be slow in the environmental pH range (4-9).

The partition coefficient of the chemical has not been determined. A calculated partition coefficient (log P) of 9.56 was determined for the chemical using the atom/fragment contribution method developed by Syracuse Research Corporation (2). Calculation of log P using ASTER gave a value of 9.38 (1).

No data has been provided on the adsorption/desorption behaviour of the notified product. Calculation of Log K_{OC} using ASTER gave values of 6.44 (1). Hence, the chemical is likely to strongly adsorb to soils and sediments.

The notified chemical does not contain acidic or basic functional groups which could gain or lose a proton in the environmental pH range (4-9).

4. PURITY OF THE CHEMICAL

Degree of Purity: 99.9%

Toxic or Hazardous Impurities: none

Non-hazardous Impurities (> 1% by weight): none

Additives/Adjuvants: none

5. USE, VOLUME AND FORMULATION

The notified chemical will not be manufactured in Australia. Isostearene will be imported at 5% w/w of a formulated finished product. It will be used as a moisturising day cream for topical application in small quantities at one time. Isostearene will be used as an emollient (skin conditioning agent). It will act as a lubricant on the *stratum corneum* to reduce and improve the skin appearance.

There will not be any reformulation of the product containing the notified chemical in Australia.

It is estimated that less than 1 000 kg of the notified chemical will be imported per annum for the next five years.

6. OCCUPATIONAL EXPOSURE

The notified chemical will be imported as an ingredient of a moisturising day cream formulation packed in 100 mL enclosed plastic jars. Each jar will be placed in a carton. Six cartons are then shrink wrapped and packed into cardboard shippers.

Upon receipt of the finished product containing the notified chemical in Australia, 2 to 3 warehouse workers will handle and transfer the product packed in cardboard shippers from wharf to road transport vehicles. It will then be transported to Johnson & Johnson Pacific warehouse at Botany for storage at ambient temperature.

The notified chemical containing the product will be transported directly from Johnson & Johnson Pacific warehouse to retail outlets (supermarkets and chemists).

There should is not be any exposure to the notified chemical during storage and distribution, except in the event of a spill.

7. PUBLIC EXPOSURE

The level of the notified chemical in the cream is 5%. Since it is used in a cosmetic moisturising cream, the major public exposure will occur by the dermal route. Public exposure from transport, storage and disposal is expected to be negligible.

8. ENVIRONMENTAL EXPOSURE

Release

Under normal conditions, the chemical within the finished products would not be released during storage and transportation.

The use of creams containing the chemical would be widespread but diffuse as they would be applied in small quantities to the skin. Release to the environment may occur to the sewer or to landfill through the removal of the cream from the skin by washing or wiping, and the disposal of residual quantities of the cream within used containers. The notifier claims that due to the chemical's strong affinity with the skin, not more than 0.1% of the product will be lost to the sewer through normal use. This would release approx 1 kg of the notified chemical through washing to effluent. Assuming 0.5% remains in containers, another 5 kg would be released to the environment through disposal in landfill.

Fate

The notified chemical is intended for use in cosmetics. It would be released to the environment via consumer use either through landfill of discarded paper or cotton wipes or through washing the residual chemical off the skin and into the sewerage system.

No biodegradation data have been provided. While this is not required by the Act for chemicals imported at volumes of less than one tonne per annum, the chemical is of a type that could be susceptible to biodegradation since it is composed of a long chain aliphatic alcohol esterified with lauric acid. However, the low solubility would be likely to inhibit degradation. The biodegradability is supported by QSAR calculations using ASTER, which estimates a biological oxygen demand (BOD) half-life of between 2 and 16 days (1). The molecular weight and high log K_{OW} of the chemical indicates that it could potentially bioaccumulate (3). This is confirmed by the determination of a value of 100 000 for the bioconcentration factor (BCF) using QSAR calculations (1). However, the potential for bioaccumulation is decreased by the low water solubility of the chemical and its expected metabolism by aquatic organisms and low exposure to the aquatic compartment.

Level 1 Mackay calculations for the notified chemical performed using ASTER (1) indicate that, at equilibrium, approximately 0.02%, 0.00%, 0.03%, 0.08%, 48.21% and 51.65% will be partitioned to air, water, aquatic biota, suspended solids, sediment and soil, respectively.

9. EVALUATION OF TOXICOLOGICAL DATA

Summaries only of toxicological data were provided. The full test reports were not requested.

9.1 Acute Toxicity

Summary of the acute toxicity of Isostereane

Test	*Species*	*Outcome*	*Reference*
acute oral toxicity	rat	LD_{50} > 13 000 mg/kg	(4)
intraperitoneal toxicity	rat	LD_{50} > 8620 mg/kg	(5)
skin irritation (30% in liquid paraffin)	rabbit	non irritant	(6)
eye irritation (10% in liquid paraffin)	rabbit	non irritant	(8)
skin sensitisation	guinea pig	non sensitiser	(9)

9.1.1 Oral Toxicity (4)

Species/strain:	rat/Wistar White
Number/sex of animals:	not provided
Observation period:	not provided
Method of administration:	a single dose of 13 000 mg/kg (> 15 mL/kg) of the test substance administered by gavage
Clinical observations:	not provided
Mortality:	none recorded
Morphological findings:	none recorded
Test method:	not provided
LD_{50}:	> 13 000 mg/kg
Result:	the notified chemical was of very low acute oral toxicity in rats

9.1.2 Intraperitoneal Toxicity (5)

Species/strain:	mice/Swiss
Number/sex of animals:	5/sex
Observation period:	not provided
Method of administration:	intraperitoneal
Clinical observations:	not provided
Mortality:	not provided
Morphological findings:	not provided
Test method:	not provided
LD_{50}:	> 8620 mg/kg (> 10 mL/kg)
Result:	the notified chemical was of low acute intraperitoneal toxicity in mice

9.1.3 Inhalation Toxicity not provided

9.1.4 Skin Irritation (6)

Species/strain:	rat/Wistar
Number/sex of animals:	not provided/male
Observation period:	not provided
Method of administration:	topical; on two 4 cm^2 test sites (intact and scarified) of the dorsal skin; dose level 500 mg for each site, 30% in liquid paraffin
Test method:	FDA (7)
Result:	the notified chemical was not irritating to the skin of rabbits

9.1.5 Eye Irritation (8)

Species/strain:	rabbit/New Zealand White
Number/sex of animals:	not provided
Observation period:	not provided
Method of administration:	10% in liquid paraffin
Test method:	FDA (9)
Result:	no significant treatment-related ocular lesions

9.1.6 Skin Sensitisation (9)

Species/strain:	guinea pig/Dunkin Hartley White
Number of animals:	not provided
Induction procedure:	not provided (route dermal)
Challenge procedure:	not provided (route dermal)
Challenge outcome:	no skin reactions were observed at 24 and 48 hour time intervals after the challenge

Test method:	Magnusson and Kligman maximisation test (10)
Result:	the notified chemical was non-sensitising to the skin of guinea pigs

9.2 28-Day Repeated Dose Toxicity (11)

Species/strain:	rat/Wistar
Number/sex of animals:	not provided/males and females
Method of administration:	oral (details not provided)
Dose/Study duration::	500, 1 500 and 4 500 mg/kg/day; 6 days a week for 4 successive weeks
Clinical observations:	not provided
Clinical chemistry/Haematology	not provided
Histopathology:	not provided
Test method:	(12)
Result:	no treatment-related changes were observed up to 4 500 mg/kg/day of the test substance

9.3 Genotoxicity

9.3.1 *Salmonella typhimurium* Reverse Mutation Assay (13)

Strains:	Salmonella typhimurium TA 97, TA 98, TA 100 and TA 102
Concentration range:	312 to 5 000 µg/plate
Test method:	Ames et al. (14)
Result:	there was no significant increase in revertant colony numbers

9.4 Overall Assessment of Toxicological Data

The assessment is based on the summary data provided in the submission. The test substance exhibited very low acute toxicity in rats by oral administration (LD_{50} > 13 000 mg/kg) and intraperitoneal administration (LD_{50} > 8 620 mg/kg). The notified chemical was non-irritant to the skin and eye of rabbit, when tested at 30% and 10% in liquid paraffin, respectively. It was not a skin sensitiser in guinea pigs.

In a 28-day repeat oral dose toxicity study in rats, the notified chemical did not exhibit any treatment related changes.

The notified chemical was found not to be mutagenic *in vitro* by bacterial reverse mutation assay.

According to the NOHSC *Approved Criteria for Classifying Hazardous Substances* (15), the notified chemical would not be classified as hazardous, in relation to the toxicological end points measured.

10. ASSESSMENT OF ENVIRONMENTAL EFFECTS

No ecotoxicological data were provided.

11. ASSESSMENT OF ENVIRONMENTAL HAZARD

The hazard posed by the moisturising creams containing the notified chemical appears to be low as the chemical will be incorporated at a small percentage (5%) and the use of the creams is expected to be spread out across Australia. Release of the notified chemical to the environment may occur through the use within moisturising creams. Most of this is expected to be consigned to landfill after removal from the body by paper tissues or cotton wool.

Taking the worst case assumption that 10% of the imported chemical remains suspended in the sewerage system and is discharged to receiving waters, a predicted environmental concentration (PEC) for the substance in sewage water across Australia can be estimated from the following assumptions: 1 000 kg maximum annual use, an Australian population of 18 million and a daily per capita waste water discharge (a conservative estimate) of 150 L. This provides a PEC of approximately 0.01 ppb in sewage water.

This neglects adsorption to particles and sediments, which is expected to be extensive. The notified chemical has a low solubility in water and will be effectively removed during the water treatment process. Hence, it will be handled as part of the normal solid waste recovery and disposed of to approved landfill or incinerated along with residues on paper tissues and cotton wool. Thus, there is little likelihood of the notified chemical entering natural waterways in significant quantities.

A small amount (less than 5 kg per annum), the residue from 'empty' cosmetic containers, will go into landfill where based on its low water solubility it is not expected to be mobile.

The overall environmental hazard of the chemical can be rated as low.

12. ASSESSMENT OF PUBLIC AND OCCUPATIONAL HEALTH AND SAFETY EFFECTS

The notified chemical is of sufficiently low molecular weight (340.57) and lipid solubility (log P_{ow} = 9.56 estimated) to be able to penetrate the skin and other biological membranes, and hence be available for systemic absorption.

Based on the toxicological data, the notified chemical is likely to exhibit very low acute and chronic systemic toxicity, is not likely to be a skin or eye irritant nor a skin sensitiser and is not likely to be genotoxic. The notified chemical would not be classified as hazardous according to NOHSC *Approved Criteria for Classifying Hazardous Substances* (15) in relation to the available toxicity data considered in this assessment.

Exposure of workers to the notified chemical during transport and storage could only occur in the case of an accident spill where the packaging were breached. In this case dermal contact with the formulated notified chemical may occur. Exposure under these conditions would not cause any health effects to workers. No other occupational exposure is anticipated since the product containing the notified chemical is directly sold to the public from retail outlets.

Since the notified chemical will be used in a cosmetic moisturising cream, widespread public exposure will occur by the dermal route. The acute toxicity profile of the notified chemical indicates minimal acute hazards for the indicated use.

Assuming that 1 mg/cm^2 of the cream is used per application, 2 applications/day, surface areas of 840 cm^2 for both hands (front and back) and 1 180 cm^2 for the face, the amount of the notified chemical at 5% in the Johnson & Johnson Moisturising Day Cream applied on the skin would be 202 mg/day. The dermal dose for an average 60 kg person would be 3.4 mg/kg/day. This gives a safety margin of greater than 1 300, based on the oral NOEL of 4 500 mg/kg/day, which was the highest dose administered in a 28-day rat study. In practice, the safety factor probably would be higher, given that absorption through the skin is likely to be less extensive than via the oral route. The proposed use is not expected to pose a significant hazard to public health.

13. RECOMMENDATIONS

To minimise occupational exposure to the notified chemical the following guidelines and precautions should be observed:

- Spillage of the notified chemical should be avoided. Spillages should be cleaned up promptly with absorbents which should be put into containers for disposal;
- Good personal hygiene should be practised to minimise the potential for ingestion;
- A copy of the Material Safety Data Sheet (MSDS) should be easily accessible to employees.

14. MATERIAL SAFETY DATA SHEET

The MSDS for the notified chemical was provided in accordance with the *National Code of Practice for the Preparation of Material Safety Data Sheets* (16).

This MSDS was provided by the applicant as part of the notification statement. It is reproduced here as a matter of public record. The accuracy of this information remains the responsibility of the applicant.

15. REQUIREMENTS FOR SECONDARY NOTIFICATION

Under the Act, secondary notification of the notified chemical 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

1. US EPA (1998) ASTER Ecotoxicity profile: isodecyl laurate. United States Environmental Protection Agency, Office of Research and Development, National Health and Environmental Effects Research Laboratory, Mid-Continent Ecology Division. Telnet address: ecotox.epa.gov.

2. Syracuse (1998), Log Kow program, Syracuse Research Corporation, Internet address: http://esc.syrres.com

3. Connell DW (1989) General characteristics of organic compounds which exhibit bioaccumulation. In: Connell DW ed, Bioaccumulation of Xenobiotic Compounds. CRC Press, Boca Raton, USA.

4. data on file

5. data on file

6. data on file

7. Test for Primary Skin Irritants Recommended by the Food and Drug Administration Federal Register USA 37 [244]: 27035, 1972.

8. data on file

9. data on file

10. Magnusson and Kligman maximisation test (Allergic Contact Dermatitis in the Guinea Pig, Charles and Thomas, Springfield 1970.

11. data on file

12. Good Laboratory Practice (GLP) regulations

13. data on file

14. Ames et al. Mutat. Res. 31:347-364, 1975

15. National Occupational Health and Safety Commission (1994), *Approved Criteria for Classifying Hazardous Substances [NOHSC:1008(1994)]*, Australian Government Publishing Service, Canberra.

16. National Occupational Health and Safety Commission (1994), *National Code of Practice for the Preparation of Material Safety Data Sheets [NOHSC:2011(1994)]*, Australian Government Publishing Service, Canberra.