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NATIONAL INDUSTRIAL CHEMICALS NOTIFICATION AND ASSESSMENT SCHEME

FULL PUBLIC REPORT

NONANOIC ACID, POTASSIUM SALT

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Director
Chemicals Notification and Assessment

FULL PUBLIC REPORT

NONANOIC ACID, POTASSIUM SALT

1. APPLICANT

Kodak Australasia Pty Ltd, 173 Elizabeth Street, Coburg, Victoria, 3058

2. IDENTITY OF THE CHEMICAL

Chemical name:	Nonanoic acid, potassium salt
Chemical Abstracts Service (CAS) Registry No.:	23282-34-0
Other name(s):	Potassium nonanoate Pelargonic acid, potassium salt
Trade name(s):	None
Molecular formula:	$C_9H_{18}O_2K$
Structural formula:	$CH_3-(CH_2)_7-COOK$
Molecular weight:	197.34

Method of detection and determination:

Spectral data: (nonanoic acid. sodium salt) major IR peaks at 1430, 1450, 1560 and 2940 cm^{-1}

3. PHYSICAL AND CHEMICAL PROPERTIES

Appearance at 20°C and 101.3 kPa:	Clear liquid (in solution)
Melting Point:	250°C (nonanoic acid sodium salt)

Density:	1170 kg/m^3 at 25°C (octanoic acid, potassium salt)
Vapour Pressure:	Not available
Water Solubility:	Saturation point not determined. An aqueous solution of 18 g/100 mL at 90°C has been reported for the sodium salt (1). The sodium salt forms complex solutions that may contain free ionic and neutral molecules as well as ionic and neutral micelles. Similarly, nonanoic acid, potassium salt would be expected to be essentially miscible with water.
Hydrolytic Stability:	Data not available. Neutralisation to the stable free acid would be expected at low pH.
Partition Co-efficient (n-octanol/water) log $P_{O/W}$:	Not available. This is not relevant for compounds which dissociate in solution. Salts of aliphatic carboxylic acids are not expected to be lipophilic.
Adsorption/Desorption:	Not available
Dissociation Constant:	Not available. Solutions expected to be alkaline. The pH of a 0.1 M aqueous solution of sodium acetate at 25°C is 8.9.
Flash Point:	Not available
Flammability Limits:	Not available

Decomposition Temperature: Not available

Autoignition Temperature: Not available

Explosive Properties: Not available

Reactivity/Stability: Not available

Particle size distribution: Not available
(The chemical will be imported as an aqueous solution.)

4. PURITY OF THE CHEMICAL

Degree of purity: Approximately 94%

Toxic or hazardous impurity/impurities: None

Non-hazardous impurity/impurities: (> 1% by weight)

. **Chemical name:** Octanoic acid, potassium salt
CAS No.: 764-71-6
Weight percentage: 4%

. **Chemical name:** Decanoic acid, potassium salt
CAS No.: 13040-18-1
Weight percentage: 2%

Additive(s)/Adjuvant(s): None

5. INDUSTRIAL USE

Nonanoic acid, potassium salt will be imported as a component of the aqueous developer solution, MX-1587-1, which will be used in aqueous lithographic plate processing in the printing industry.

It is estimated that 700 kg of nonanoic acid potassium salt will be imported in the first year.

6. OCCUPATIONAL EXPOSURE

The aqueous developer solution, MX-1587-1, containing nonanoic acid, potassium salt will be transported and stored in polyethylene drums (5 US Gallons).

The notified chemical in the developer solution will be distributed by Kodak to about 150 commercial printing establishments in Australia. At each establishment 1-2 people will be involved in manual handling of the developer solution. The developer solution will be either poured or pumped directly into the Automatic Plate Processor holding tanks.

Almost all of the lithographic plate processing in Australia is conducted in a closed system using a 3-bath automated plate processor consisting of the following three phases:

1. development (closed loop recirculation)

2. water wash (either closed loop or flush-to-sewer); and

3. "gumming" (closed loop recirculation).

7. PUBLIC EXPOSURE

Nonanoic acid, potassium salt contained in the lithographic plate developer, MX-1587-1 will only be supplied to commercial printing establishments and will not be available to the public. Although no information on the binding of the notified chemical to the final printed product has been provided, transfer of the notified chemical to the printed product, and therefore public exposure, is expected to be negligible. The potential for public exposure as a result of disposal to sewer is expected to be low.

8. ENVIRONMENTAL EXPOSURE

. Release

The principal route of environmental exposure will be through disposal of diluted and spent solutions to sewer. Each m^2 of plate processed requires the addition of 50 mL of MX 1587-1

(3.5 g notified substance) to the development tank. Automatic processors operate at up to 2 m per minute (plates are approx 1 m wide) with cycle times around 3.5 minutes and water consumption 7-8 L per minute. At the maximum processing speed of 2 m per minute, the concentration of notified substance leaving the processor would be 7 g in 7 L, or 1000 ppm. The material safety data sheet indicates that spills will also be flushed to sewer with large amounts of water. Neutralisation will convert the notified substance to the free acid, which is listed on AICS.

. Fate

Biodegradability testing is not required for small volume notifications. However, fatty acids and their salts are recognised as being easily biodegradable (2). Biodegradation occurs enzymatically, with beta-oxidation by lipases leading to cleavage of the hydrocarbon chain. In standard dilute sewage, nonanoic acid has a 5 d BOD of 0.59, approximately 20% of theoretical (3). This indicates that partial degradation should occur during sewage treatment, and that residues should not persist in the environment.

Removal of soaps from sewage treatment works and aquatic environments also occurs through precipitation as the insoluble calcium and magnesium salts.

9. EVALUATION OF TOXICOLOGICAL DATA

No toxicity data are required under the *Industrial Chemicals (Notification and Assessment) Act 1989* for chemicals which are to be introduced in quantities of less than 1000 kg per year. Thus, no toxicity data on nonanoic acid, potassium salt were submitted. A search of the literature also did not reveal any toxicity data on the notified chemical. However, some summary toxicity data was submitted for nonanoic acid, and further data was found in the literature on the toxicity of salts of other longchain aliphatic carboxylic acids.

9.1 Acute Toxicity

Table 1: Summary of the acute toxicity of nonanoic acid.

Test	Route	Species	Outcome	Ref.
Acute toxicity (undiluted material)	Oral	Rat	LD_{50} > 3200 mg/kg	(4)
Acute toxicity (undiluted material)	IP*	Rat	LD_{Lo} = 3200 mg/kg	(4)
Acute toxicity (undiluted material)	IV+	Mouse	LD_{50} = 224 mg/kg	(5)
Acute toxicity (10% in corn oil)	Oral	Mouse	LD_{50} > 3200 mg/kg	(4)
Acute toxicity (10% in corn oil)	IP*	Mouse	LD_{Lo} = 1600 mg/kg	(4)
Acute toxicity	Dermal	Rabbit	LD_{50} > 5000 mg/kg	(5)

* IP = Intraperitoneal
\+ IV = Intravenous

9.1 Acute Toxicity

There were no deaths when nonanoic acid was administered orally to rats at a dose of 3200 mg/kg (4). However deaths did occur at this dose level when the chemical was administered intraperitoneally (4). Nonanoic acid administered to mice by the intravenous route had an LD_{50} of 224 mg/kg (5). A 10% solution of nonanoic acid in corn oil failed to kill mice at dose of 3200 mg/kg when given orally, but caused death at a dose of 1600 mg/kg by the intraperitoneal route. Symptoms in mice included laboured respiration and roughing of the coat, death was observed as long as 4 days after dosing (4). The dermal LD_{50} for nonanoic acid in rabbits has been reported to be > 5000 mg/kg (5).

These data show that nonanoic acid has low acute toxicity by the intravenous, intraperitoneal, oral or dermal routes. Therefore, the potassium salt would also be expected to have low acute toxicity.

9.2 Skin Irritation

Solutions of nonanoic acid at 0.5 M or 1.0 M in propanol caused skin irritation in 25 human volunteers when applied under occlusive patches (5). Similarly, 20% nonanoic acid solution in propanol produced skin reactions in 94% of the 116 healthy male volunteers who were patch tested. The lesions consisted of mainly erythema at 48 hours and pigmentation at 96 hours (6).

Nonanoic acid, left in contact with the skin for 24 hours, was found to be a moderate skin irritant in rabbits treated at 500 mg/kg (5). The same chemical in an undiluted form produced severe skin irritation in guinea pigs when applied to the skin (5).

9.3 Eye Irritation

Severe irritation was produced by the application of 91 mg of nonanoic acid to the rabbit eye (5).

9.4 Respiratory Irritation

Rats exposed to atmospheric concentrations of 840 mg/m^3 (125 ppm) for a period of 6 hours showed no symptoms of toxicity. However, in another study, test animals (species not specified) were subjected to an atmospheric concentration of 3.75 mg/L (1150 ppm) for a period of 6 hours. Clinical signs were nasal discharge, blinking, and laboured breathing (4).

Inhalation exposure indicated nonanoic acid to be a respiratory irritant.

9.5 Skin Sensitisation

No sensitisation reactions could be observed in 25 human volunteers after patch testing with 12% nonanoic acid solution in petroleum ether (5).

9.6 Mechanistic Studies

9.6.1 Skin Irritation

The effects of a series of sodium salts of aliphatic carboxylic acids (C8, C10, C12, C14 and C16) on DNA synthesis in guinea-pig kidney fibroblasts, the release of histamine from isolated rat peritoneal mast cells and the release of cytoplasmic proteins from guinea-pig kidney fibroblasts have been studied as a model for the irritant effects of such compounds (7). The C12 compound was the most potent in the series in inhibiting DNA synthesis (0.1 mM) and inducing histamine (0.4 mM) and protein (7.1 mM) release. The order of potency was C12 > C14 > C16 > C10 > C8.

9.6.2 Inhibition of Transport Across Membranes

Octanoic acid, sodium salt at 5 mmol/kg administered intravenously to rhesus monkeys induced a 20-minute coma with myoclonia followed by complete muscular atony and disappearance of ocular movements (8). At the same dose, a clinical and electroencephalographic syndrome resembling hepatic encephalopathy was observed in 5 rhesus monkeys (9).

Octanoic acid, sodium salt at a concentration of 0.2 M was administered to rabbits by slow intravenous infusion over 4 hours. Significant inhibition of regional Na/K-ATPase activity was detected in the cortex, thalamus, hypothalamus, pons and medulla (10).

Octanoic acid, sodium salt at a concentration of 4.4 mmol modified the intracellular action potential in isolated rabbit atrium and papillary muscle. The rate of depolarisation and time of repolarisation were markedly decreased, while there was no change in the resting membrane potential. The amplitude of the action potential and reverse potential showed moderate decreases (11).

In another study, a series of sodium salts of aliphatic carboxylic acids (C3, C4, C5, C6 and C8) were tested for their effects on sodium transport by the toad bladder. Low concentrations (0.1 - 1.0 mmol) stimulated sodium transport, while higher concentrations (5 - 20 mmol) reversely inhibited sodium transport (12).

Octanoic acid, sodium salt at a concentration of 0.37 µmol decreased the incorporation of L-leucine into normal rat liver slices and hepatoma cells by approximately 75% (13).

Overall, these data indicate that octanoic acid sodium salt may be interfering with transport across the cell membrane.

9.6.3 Platelet Aggregation

Intravenous administration of octanoic acid, sodium salt to rabbits (dose not specified) resulted in a pronounced, although transient, inhibition of platelet adhesiveness. A single oral dose had no effect on platelet adhesiveness, while repeated oral dosing (up to 3 weeks) resulted in progressive and significant decrease in platelet adhesiveness (14).

9.7 Overall Assessment of Toxicological Data

No toxicity data on nonanoic acid potassium salt were submitted. The toxicity profile of the notified chemical would be expected to be similar to that of closely related compounds. Some toxicity data on nonanoic acid, the parent compound, was submitted and additional data on octanoic acid, sodium salt were available in the literature.

Nonanoic acid has low acute toxicity via the oral and dermal routes. The LD_{50} values for nonanoic acid potassium salt, administered by the intravenous or intraperitoneal route also indicate that this substance has a relatively low acute toxicity.

Nonanoic acid was shown to be a primary skin irritant in both humans and animals. It was found to cause moderate skin irritation in rabbits and severe skin irritation in guinea pigs. Severe eye irritation in rabbits was also observed with nonanoic acid. There was no evidence of skin sensitisation with nonanoic acid in human patch testing.

A homologous series of sodium salts of aliphatic carboxylic acids (C8, C10, C12, C14 and C16) were found to inhibit DNA synthesis and cause the release of protein from fibroblasts. These compounds also induced histamine release from mast cells.

Several studies on octanoic acid, sodium salt indicated that it had the potential to interfere with transport across the cell membrane.

Octanoic acid, sodium salt was shown to inhibit platelet adhesiveness in vivo.

10. ASSESSMENT OF ENVIRONMENTAL EFFECTS

Environmental effects testing is not a requirement for low volume chemicals. However, the aquatic toxicity of nonanoic acid potassium salt may be estimated by comparison with the free acid and its sodium salt, for which quantitative structure activity realtionships have been developed (15). Fatty acid sodium salts were found to be less toxic than the parent acids, and toxicities of both increased with chain length (between 6 and 12 carbons). For capric acid (C10) in fresh water, the 48 h LC_{50}s to red killifish (*Oryzias latipes*) and gammarus (*Hyale plumulosa*) were 20 and 41 $mg.L^{-1}$, respectively. Sodium caprate was less toxic than the acid to killifish (54 $mg.L^{-1}$). Based on these data, nonanoic acid potassium salt would be expected to be no more than slightly toxic to aquatic fauna.

Toxicity to algae may be estimated by comparison with data for soaps in general. For example, a range of 180-320 $mg.L^{-1}$ has been reported for *Chlorella vulgaris* (2). Nonanoic acid, potassium salt would therefore not be expected to be significantly toxic to algae.

11. ASSESSMENT OF ENVIRONMENTAL HAZARD

For 150 customers, the estimated import volume corresponds to around 5 kg per customer per year, or a daily use per establishment of 20 g, assuming each processor operates for 250 d per year. In a hypothetical worst case situation of 10 such customers discharging to a rural sewage treatment works with a daily flow of 5 ML, the concentration of notified substance in the effluent would be reduced to 40 ppb simply by dilution, and further by any degradation or sorption that occurs.

In view of the low aquatic toxicity predicted for nonanoic acid potassium salt and lack of bioaccumulation potential, the

environmental hazard associated with the proposed lithographic use would appear negligible.

12. ASSESSMENT OF PUBLIC AND OCCUPATIONAL HEALTH AND SAFETY EFFECTS

No toxicity data were provided for nonanoic acid potassium salt. However, the notified chemical would be expected to have a similar toxicity profile to nonanoic acid and salts of aliphatic carboxylic acids of similar chain length. Nonanoic acid, potassium salt would be expected to have low oral and dermal acute toxicity, be a primary skin and eye irritant, able to interfere with transport across the cell membrane, and reduce platelet adhesiveness. Thus, oral exposure and eye and skin contact with the notified chemical should be avoided.

The use pattern indicates that occupational and public exposure to nonanoic acid, potassium salt will be minimal under normal use conditions. Therefore, the notified chemical would be expected to be of low hazard to human health.

13. RECOMMENDATIONS

To minimise occupational exposure (and public/environmental if recommendations have been made by these agencies) to nonanoic acid, potassium salt the following guidelines and precautions should be observed:

- If engineering controls are insufficient to reduce exposure to a safe level, the following personal protection equipment should be worn, as the notified chemical is a severe eye and moderate skin irritant:
  - face shield (AS 1336 and AS 1337) (16,17);
  - impervious gloves (AS 2161) (18);
  - protective clothing (AS 3765.1, AS 3765.2) (19,20);
- good work practices should be implemented to avoid spillages or splashings and in the case of handling nonanoic acid, potassium salt and the formation of a mist;
- Any spillages should be promptly cleaned up and disposed according to local or state regulations;

. good personal hygiene should be observed; and

. a copy of the Material Safety Data sheet for nonanoic acid, potassium salt and products containing it should be easily accessible to workers.

14. MATERIAL SAFETY DATA SHEET

The Material Safety Data Sheet (MSDS) for nonanoic acid, potassium salt (Attachment 1) was provided in Worksafe Australia format (21). This MSDS was provided by Kodak Australasia 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 Kodak Australasia Pty Ltd.

15. REQUIREMENTS FOR SECONDARY NOTIFICATION

Under the *Industrial Chemicals (Notification and Assessment) Act 1989* (the Act), secondary notification of nonanoic acid potassium salt 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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18. Australian Standard 2161-1978, Industrial Safety Gloves and Mittens (excluding Electrical and Medical Gloves), Standards Association of Australia Publ., Sydney, 1978.

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