



**Australian Government**

**Department of Health and Aged Care**

Australian Industrial Chemicals Introduction Scheme

# **Carbonodithioic acid, O-(2-methylbutyl) ester, sodium salt (1:1)**

**Assessment statement (CA09899)**

**14 June 2024**



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# AICIS assessment (CA09899)

## Chemical in this assessment

Name	CAS registry number
Carbonodithioic acid, O-(2-methylbutyl) ester, sodium salt (1:1)	72187-33-8

## Reason for the assessment

An application for an assessment certificate under section 31 of the *Industrial Chemicals Act 2019* (the Act).

### Certificate Application type

AICIS received the application in a Health and Environment Focus type.

## Defined scope of assessment

The chemical has been assessed:

- as manufactured in Australia as an aqueous solution at up to 1,000 tonnes per year at up to 40% concentration
- for use by professional workers in industrial mining facilities as a flotation agent at up to 8% concentration in aqueous solution

## Summary of assessment

### Summary of introduction, use and end use

The assessed chemical will be manufactured in Australia at up to 1,000 tonnes per year at up to 40% concentration in aqueous solution for local use. After manufacture, the solution containing the assessed chemical will be diluted with water to the desired concentration (up to 8% concentration) and stored at approximately 10 °C in readiness for dispatch. The assessed chemical at up to 8% concentration will be transported by road from the manufacturing facility directly to the end use site in 17 kL or 21 kL ISO tank containers.

The assessed chemical will only be used in industrial mining facilities as a flotation agent for metal extraction. There will be no consumer use of products containing the assessed chemical. The extraction fluid will contain the assessed chemical at up to 8% concentration.

### Human health

#### Summary of health hazards

The submitted toxicological data on analogue chemicals (see **Supporting information**) indicate that the assessed chemical is:

- of moderate acute oral toxicity at 10% concentration (median lethal dose (LD50) = 730 mg/kg bw in mice)
- corrosive to the skin
- a skin sensitiser
- not genotoxic.

Repeated dose oral and inhalation toxicity studies on analogue chemicals indicate that the assessed chemical can produce systemic adverse health effects following repeated oral and inhalation exposure. Sub-chronic repeated dose oral toxicity studies on an analogue chemical reported effects on the central nervous system, liver and spleen with a lowest observed adverse effect level (LOAEL) of 10 mg/kg bw/day in rats. Similarly, a sub-chronic repeated dose inhalation toxicity study on an analogue chemical reported effects on the central nervous system, liver and kidneys of mice, with a lowest observed adverse effect concentration (LOAEC) of 100 mg/m<sup>3</sup>.

### Hazard classifications relevant for worker health and safety

Based on the data provided by the applicant on analogue chemicals, the assessed chemical satisfies the criteria for classification according to the *Globally Harmonized System of Classification and Labelling of Chemicals* (GHS) (UNECE 2017) for hazard classes relevant for worker health and safety as adopted for industrial chemicals in Australia.

Health hazards	Hazard category	Hazard statement
Acute toxicity – oral*	Category 4	H302: Harmful if swallowed
Skin corrosion	Category 1	H314: Causes severe skin burns and eye damage
Skin sensitisation	Category 1	H317: May cause an allergic skin reaction
Specific target organ toxicity - repeated exposure	Category 2	H373: May cause damage to organs through prolonged or repeated oral and inhalation exposure

\* Based on 10% solution of analogue chemical

### Summary of health risk

#### Public

The products containing the assessed chemical will not be available for use by the public. When introduced and used in the proposed manner, it is unlikely that the public will be exposed to the chemical.

This assessment does not identify any risks to public health that require specific risk management measures.

## Workers

Limited operational exposure is expected during manufacturing, reformulation, and end use applications due to the use of engineering/enclosed systems. Only trained personnel will be transferring the assessed chemical from bulk containers to containment tanks at industrial sites and the applicant has also indicated that it is mandatory for workers to wear personal protective equipment (PPE) such as protective clothing and footwear, impervious gloves, face shield, goggles and hard hat.

Considering the critical health effects possible through exposure to the assessed chemical, control measures to minimise dermal, ocular and inhalation exposure are needed to manage the risk to workers (see **Means for managing risk section**).

## Environment

### Summary of environmental hazard characteristics

According to domestic environmental hazard thresholds and based on available data, the assessed chemical is:

- Persistent (P)
- Not Bioaccumulative (Not B)
- Toxic (T)

### Environmental hazard classification

The assessed chemical satisfies the criteria for classification according to the *Globally Harmonized System of Classification and Labelling of Chemicals* (GHS) (UNECE 2017) as Acute Category 1 (H400) and Chronic Category 1 (H412) based on the toxicity data for fish and invertebrates. Considerations were also made for the rapid degradation of the assessed chemical.

Environmental Hazard	Hazard Category	Hazard Statement
Hazardous to the aquatic environment (acute / short-term)	Aquatic Acute 1	H400: Very toxic to aquatic life
Hazardous to the aquatic environment (long-term)	Aquatic Chronic 3	H412: Harmful to aquatic life with long lasting effects

### Summary of environmental risk

The assessed chemical will be introduced for use as a flotation agent in industrial mining facilities.

Any used/residue process flow containing the assessed chemical will be captured and disposed of to a licensed tailings facility which is designed to retain and recover all water. As such, no water containing the assessed chemical is expected to be released to the environment.

When the assessed chemical is used and disposed of in accordance with existing federal, state or territory legislations, the amounts released to the environment are expected to be negligible based on its use patterns. Correspondingly, as no direct release to the surface waters or sewers is expected from the use of the assessed chemical, a PEC for the assessed chemical has not been calculated.

The assessed chemical is readily biodegradable and hydrolytically unstable under environmental conditions. However, its major decomposition product, carbon disulfide (CS<sub>2</sub>), is expected to partition to and persist in the air compartment. Hence based on the formation of persistent degradants, the assessed chemical is considered persistent.

Although the assessed chemical is persistent and toxic according to the Australian Environmental Criteria for Persistent, Bioaccumulative and/or Toxic Chemicals (DCCEEW 2022), it does not meet all three PBT criteria.

Based on available information, the assessed chemical will have limited bioavailability and negligible environmental exposure from its use patterns. Therefore, on the basis of low hazard and limited exposure, the risk from the assessed chemical can be managed.

## Means for managing risk

### Workers

#### Recommendation to Safe Work Australia

- It is recommended that Safe Work Australia (SWA) update the *Hazardous Chemical Information System* (HCIS) to include classifications relevant to work health and safety (see **Hazard classifications relevant for worker health and safety**).

#### Information relating to safe introduction and use

The information in this statement, including recommended hazard classifications, should be used by a person conducting a business or undertaking at a workplace (such as an employer) to determine the appropriate controls under the relevant jurisdiction Work Health and Safety laws.

- The following control measures could be implemented to manage the risk arising from exposure to the assessed chemical during manufacture and use:
  - Use of engineering controls such as
    - Enclosed and automated systems
    - Adequate workplace ventilation to avoid accumulation of mists or aerosols
  - Use of safe work practices to
    - Avoid contact with skin and eyes
    - Avoid inhalation of mists or aerosols
  - Use of personal protective equipment (PPE)
    - Impervious gloves
    - Protective clothing
    - Protective footwear
    - Safety glasses/goggles or face mask

- Respiratory protection where local ventilation may be inadequate
- The storage of the assessed chemical should be in accordance with the *Safe Work Australia Code of Practice for Managing Risks of Hazardous Chemicals in the Workplace* (SWA 2023) or relevant State or Territory Code of Practice.
- As the assessed chemical is a skin sensitiser and respiratory sensitisation cannot be ruled out, control measures may need to be supplemented with health monitoring for any worker who is at significant risk of exposure to the chemical, if valid techniques are available to monitor the effect on the worker's health.
- A copy of the Safety Data Sheet (SDS) should be easily accessible to workers.

## Conclusions

The Executive Director is satisfied that the risks to human health or the environment associated with the introduction and use of the industrial chemical can be managed.

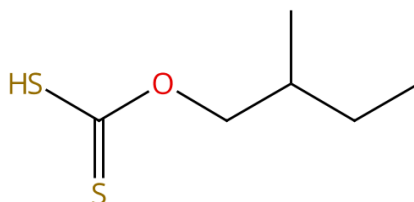
Note:

1. Obligations to report additional information about hazards under s 100 of the *Industrial Chemicals Act 2019* apply.
2. You should be aware of your obligations under environmental, workplace health and safety and poisons legislation as adopted by the relevant state or territory.

# Supporting information

## Chemical identity

<b>Chemical name</b>	Carbonodithioic acid, O-(2-methylbutyl) ester, sodium salt (1:1)
<b>CAS No.</b>	72187-33-8
<b>Molecular formula*</b>	C <sub>6</sub> H <sub>12</sub> OS <sub>2</sub> .Na
<b>Molecular weight (g/mol)*</b>	187.28
<b>SMILES (canonical)*</b>	[Na].S=C(S)OCC(C)CC
<b>Structural formula*</b>	



## Chemical description

The assessed chemical has typical purity of 8%.

\*Note: This chemical is a salt and has been represented according to CAS nomenclature/identity conventions.

## Relevant physical and chemical properties

<b>Physical form</b>	Aqueous solution	
<b>Density</b>	1.20 (relative density)	kg/m <sup>3</sup> at 20 °C
<b>Vapour pressure</b>	0.01	kPa at 25 °C
<b>Water solubility</b>	Readily soluble	
<b>Ionisable in the environment</b>	Yes	
<b>pK<sub>a</sub></b>	2.22 (calc)	



Note: assessed chemical decomposes above 25 °C and in acidic pH (NICNAS 1995) to several decomposition products, including CS<sub>2</sub>. The assessed chemical is stored at 10 °C following manufacture to limit formation of CS<sub>2</sub>.

## Introduction and use

### Workers

#### Manufacturing

The assessed chemical will be manufactured as an aqueous mixture in parallel with minor products in a fully automated batch process in a 20 kL reactor. The reactor is vented through a caustic soda scrubber and the process is controlled remotely from an enclosed control room via an automated control system. Reaction progress will be confirmed by analysis inside a fume hood in an adjacent laboratory. On completion of the batch reaction, the concentration of assessed chemical and minor products in the aqueous mixture will be approximately 40%. The solution containing the assessed chemical will be diluted with water in an enclosed system to a concentration up to 8% and stored at approximately 10 °C in readiness for dispatch to mining sites. The assessed chemical will be transported by road from the manufacturing facility directly to the end use site in 17 kL or 21 kL ISO tank containers.

#### Professional end use

At the end use site, the assessed chemical at up to 8% concentration will be delivered into a holding tank. It will be then added to a metal ore slurry to a final concentration in the parts per million range and mixed in an agitated conditioning tank. The assessed chemical/slurry mixture will then be introduced into flotation cells, where the sulphide mineral is brought to the surface by air bubbles, captured in the froth on the top of the cell and overflows into a launder from where it is pumped away for further processing.

## Human exposure

### Workers

#### Manufacturing

Transport, storage and warehouse workers are not expected to be exposed to the assessed chemical or products containing the assessed chemical, except in an unlikely event of an accidental rupture of containers. During manufacturing activities, oral, dermal, ocular and inhalational exposure to the assessed chemical at up to 40% concentration may occur, particularly where manual or open processes are used. However, according to the applicant, the use of remotely controlled, enclosed processes will limit worker exposure at the manufacturing plant.

The applicant has stated that it is mandatory for workers to wear PPE such as protective clothing and footwear, impervious gloves and safety glasses at the manufacturing facility.

## Professional end use

The applicant has indicated that there will be no manual handling of the assessed chemical during end use applications and limited operational exposure is expected due to the use of engineering/enclosed systems. Only trained personnel will be transferring the assessed chemical from bulk containers to containment tanks at industrial sites.

The applicant has further stated that it is mandatory for workers to wear PPE such as protective clothing and footwear, impervious gloves, face shield, goggles and hard hat.

## Health hazard information

The applicant has not submitted data on the assessed chemical for the toxicological endpoints. The applicant has, however, submitted toxicological data on analogue chemicals, which were appropriate for read across to the assessed chemical.

### Toxicokinetics

No toxicokinetic data were available for the assessed chemical. The class of chemicals to which the assessed chemical belongs is known to readily hydrolyse to CS<sub>2</sub> under aqueous conditions (NICNAS 1995). It is also metabolised to CS<sub>2</sub> in humans and animals (NICNAS 2000). According to the applicant, following manufacture, the assessed chemical is stored at 10 °C to limit hydrolysis to carbon disulphide.

### Acute toxicity

#### Oral

In an acute oral toxicity study (similar to OECD TG 401, conducted in 1951), groups of male albino mice were administered a 10% (w/v) solution of an analogue chemical orally by gavage (n = 13/group). The animals were observed for signs of gross toxicological effects for seven days. The majority of deaths occurred on the first day and the animals that survived appeared normal within two days. The recorded mortalities in this study were 0/13 at doses of 500 and 600 mg/kg bw, 7/13 at 750 mg/kg bw, 8/13 at 900 mg/kg bw, 9/13 at 1,000 mg/kg bw, 12/13 at 1,500 mg/kg bw, and 13/13 at 2,000 mg/kg bw. The study report did not indicate how many animals developed symptoms, at what doses and the day of development of the symptoms. The results of this study indicate that the analogue chemical at a concentration of 10% has an oral LD50 of 730 mg/kg in male mice (NICNAS 1995). Based on the results of this study, the assessed chemical at 10% concentration is likely to be of moderate acute oral toxicity, warranting hazard classification (Acute Tox. Cat. 4).

#### Observation in humans

In a case report, a worker was exposed to xanthate powder and solution (specific chemical not specified) during a mixing process at a mine site (Donoghue 1998). Extensive contamination of the chest area of the worker was evident by green staining of the skin. The worker reported gastrointestinal symptoms which began 20 hours after exposure and lasted for three days. Carbon disulfide body burden was confirmed by the detection of 2-thiothiazolidine-4-carboxylic acid in the urine (less than 4 mg/L measured approximately 68 hours after exposure). However, it was not known if the symptoms observed were caused by inhalation of CS<sub>2</sub> as a decomposition product or by dermal absorption of xanthate/carbon disulfide.

## Corrosion/Irritation

### Skin irritation

In a skin irritation study (OECD TG 404), an analogue chemical (0.5 mL) was applied undiluted to an area of clipped dorsal skin of 3 New Zealand White rabbits and covered with a semi-occlusive dressing for 4 hours. As one animal died during the first 24 hours of the test, observations from 24 hours onwards were conducted on the remaining 2 animals. Well-defined erythema (grade 4) and oedema (grade 1–2) were present at 1 hour following patch removal. Both remaining rabbits also displayed blood congestion on their skin and petechial haemorrhages were also observed in one animal. The erythema (grade 4) persisted to the 72-hour time point while the oedema worsened (grade 2–3 from 24 hours onwards). In both rabbits, a scab was also observed in the exposure area at 24, 48 and 72 hours. As there was no sign of significant reversibility, the study was terminated at 72 hours. Under the conditions of the study, the analogue chemical was determined to be corrosive to the skin, warranting hazard classification (Skin Corr. Cat. 1) for the assessed chemical.

## Sensitisation

### Skin sensitisation

The applicant did not submit any data on the skin sensitisation potential of the assessed chemical, as the assessed chemical is classified as corrosive to skin (Skin Corr. Cat. 1). The applicant has classified the assessed chemical as a skin sensitiser on a precautionary basis, as the class of chemicals to which it belongs is considered likely to be sensitising to the skin (Skin Sens. Cat. 1) (NICNAS 2017). An analogue chemical was classified as a skin sensitiser (NICNAS 2017), warranting the same hazard classification for the assessed chemical (Skin Sens. Cat. 1).

## Repeat dose toxicity

### Oral

Two non-guideline sub-chronic repeated dose oral toxicity studies on an analogue chemical have been reported (NICNAS 1995). Both studies reported similar findings, including effects on the central nervous system, liver and spleen.

In one of these studies, an analogue chemical was orally administered at 10 mg/kg bw/day to rats, rabbits and dogs for four months. From weeks 6–7 of the study, clinical effects including rapid breathing, cyanosis, hair loss and dermatitis were observed. Loss of weight and increases in blood sugar and cholesterol were observed later. From week nine of the study, convulsions and paralysis of the extremities were observed in some animals. Mortalities were observed in some animals during the study period. No further details were provided. The lowest observed adverse effect level (LOAEL) was 10 mg/kg bw/day in this study.

Although there are insufficient data to warrant classification for the assessed chemical following repeated oral exposure, potential adverse systemic effects of the assessed chemical cannot be excluded, based on analogue data. Therefore, the assessed chemical warrants hazard classification (STOT Rep. Exp. Cat. 2).

## Inhalation

In a repeated dose inhalation toxicity study (similar to OECD TG 412), Swiss Webster mice (n = 10 males/dose), SD rats (n = 10 males/dose), New Zealand White rabbits (n = 4 males/dose) and Beagle dogs (n = 2 males/dose) were exposed to an analogue chemical as aqueous aerosol (whole body) at concentrations of 0, 100 and 800 mg/m<sup>3</sup> (equivalent to actual doses of 0, 23 and 252 mg/m<sup>3</sup>) for six hours per day, five days per week for one month (20 exposures) (NICNAS 1995).

Most of the mice died when exposed to 800 mg/m<sup>3</sup>. Five of the 16 mice that died showed convulsions and hyperactivity prior to death. Higher liver to body weight ratio was observed in the mice of both treatment groups. Higher liver to body weight ratio, an increase in the absolute kidney weight (in males only), high serum alanine aminotransferase activity and microscopically visible granular degeneration of the renal tubular epithelial cells were observed in the rats of the high dose group. Marked elevations of liver enzyme activities and hepatocellular degeneration, necrosis and inflammation were observed in the dogs of both treatment groups. No effects were observed in the treated rabbits. The lowest observed adverse effect concentration (LOAEC) was 100 mg/m<sup>3</sup> in this study (NICNAS 1995).

Under the conditions of this study and based on the above findings, the assessed chemical warrants hazard classification (STOP Rep. Exp. Cat. 2).

## Genotoxicity

An analogue chemical was not mutagenic in a bacterial reverse mutation assay using *Salmonella typhimurium* strains TA98, TA100, TA1535 and TA1537 and *Escherichia coli* strain WP2uvrA (together with *Escherichia coli* WP2 (pKM101)), with presence and absence of metabolic activation (S9-mix). The Ames fluctuation assay was used which is consistent with OECD TG 471. No significant increases in the frequency of revertant colonies were recorded for any of the bacterial strains, with any tested concentration of the assessed chemical, except for *S. typhimurium* strain TA98 (without S9-mix) at a single concentration (0.016 mg/mL). However, as the increase in revertants over baseline was less than 2-fold and a dose response was absent, this result was considered by the study authors to be anomalous. Under the conditions of this study, the analogue chemical was not considered to be mutagenic either in the presence or absence of metabolic activation. Therefore, the assessed chemical is unlikely to cause point mutations.

No structural alerts for mutagenicity or clastogenicity were observed for an analogue chemical or its metabolites using QSAR software MC4PC (version 2.4.1.5) (MultiCASE Inc. 2011).

Based on the available in vitro data and in silico predictions, the assessed chemical is not considered to be genotoxic.

## Environmental exposure

The assessed chemical is manufactured locally in a batch process at a Major Hazards Facility in Kwinana, WA.

The assessed chemical is produced via a reaction process that is fully automated. The reaction mixture is then diluted to the desired concentration and stored until dispatch.

As the reaction process is fully automated any release of the assessed chemical to the environment during manufacture is expected to be minimal.

Aqueous mixture containing the assessed chemical will be added to a process plant to aid in recovery of gold/metal bearing material. The process plant is situated on secondary containment of concrete and all process flow is directed to a licensed tailings facility which is designed to retain and recover all water. When suitable precautions are taken to avoid entry of tailings to waterways, no water containing the assessed chemical is expected to be released to the environment as a result of this gold/metal recovery process.

## Environmental fate

### Partitioning

The assessed chemical is produced *in situ* and is not isolated from the aqueous solution. It is ionisable and based on information provided on analogue chemicals, it is expected to dissociate under acidic pH conditions (Institute of Energy Technology 2020; Pomianowski A and Leja J 1963).

Due to its ionisable nature, the assessed chemical is not expected to partition to and become mobile in soil compartment.

Based on submitted information on an analogue chemical, the assessed chemical is expected to be non-volatile and as such is not expected to partition to air compartment (NICNAS 2000).

### Degradation

Degradation studies of analogue chemicals in water indicate that the assessed chemical is readily biodegradable. Results of a submitted biodegradation study for two analogue chemicals showed 95.4% and 100% degradation (OECD TG 301) over 28 days, fulfilling the 10-day-window criterion.

Based on its use patterns and submitted data of analogue compounds on hydrolysis, the most likely decomposition pathway for the assessed chemical, in neutral and alkaline conditions, is expected to be hydrolysis, producing alcohols, bicarbonates and carbon disulfide (Institute of Energy Technology 2020). This reaction is shown to have a half-life of 7.5 days at pH 7, 9.5 °C. In acidic conditions, the assessed chemical is expected to dissociate (based on information provided on an analogue) and as such, it is hydrolytically unstable under environmental pH conditions.

CS<sub>2</sub> is expected to be the major decomposition product of hydrolysis and is expected to partition mainly to air compartment due to its high volatility. When in soil, it will rapidly evaporate and enter air compartment. In air, it is shown to have a half-life of 8 days based on reactions with hydroxyl radicals and hence is expected to be persistent in air compartment as it exceeds the domestic threshold of 2 days. In water, CS<sub>2</sub> is shown to have a half-life of less than 2 days and hence is considered to be non-persistent in aquatic compartment (DCCEEW 2022).

### Bioaccumulation

No bioaccumulation information was provided for the assessed chemical.

The assessed chemical is short lived in the environment. As such, it is expected to have low bioavailability and low potential to bioaccumulate in aquatic environments.

## Predicted environmental concentration (PEC)

The predicted environmental concentration (PEC) has not been calculated as release of the assessed chemical to the aquatic environment is expected to be negligible based on its assessed use patterns.

## Environmental effects

### Effects on aquatic Life

#### Acute toxicity

The following median lethal concentration (LC50) and effective concentration (EC50) values for model organisms were submitted for analogues of the assessed chemical.

Taxon	Endpoint	Method
Fish	96hr LC50 = 8.766 mg/L	<i>Notropis atherinoides</i> (Emerald shiner) Mortality EPA ECOSAR 1.1 EPA OPPT module Calculated concentration
Invertebrate	48hr EC50 = 0.908 mg/L	<i>Daphnia magna</i> (water flea) Immobility EPA ECOSAR 1.1 EPA OPPT module Calculated concentration
Algae	48hr EC50 = 0.619 mg/L	<i>Desmodesmus subspicatus</i> (green alga) Growth rate EPA ECOSAR 1.1 EPA OPPT module Calculated concentration

#### Chronic toxicity

The following median chronic value (ChV) and effective concentration (EC50) values for model organisms were supplied for the assessed chemical and analogue chemicals, respectively.

Taxon	Endpoint	Method
Fish	30 day ChV = 1.056 mg/L	<i>Oncorhynchus mykiss</i> (Rainbow trout) Mortality EPA ECOSAR 1.1 EPA OPPT module Calculated concentration

## Invertebrates

21 day EC50 = 0.372 mg/L  
(analogue)

*Daphnia magna*  
(water flea)  
Mortality  
Semi-static conditions  
Nominal concentration

### Predicted no-effect concentration (PNEC)

A predicted no-effect concentration (PNEC) of 6.19 µg/L was calculated for the assessed chemical in the aquatic environment. This value was derived using the endpoint value for 48 hr EC50 for algae (0.619 mg/L). An assessment factor of 100 was applied based on data available for acute endpoints for three trophic levels and chronic endpoints for two trophic levels (EPHC 2009).

## Categorisation of environmental hazard

The categorisation of the environmental hazards of the assessed chemical according to the Australian Environmental Criteria for Persistent, Bioaccumulative and/or Toxic Chemicals (DCCEEW 2022) is presented below:

### Persistence

Persistent (P). Based on formation of persistent degradants, the assessed chemical is categorised as Persistent.

### Bioaccumulation

Not Bioaccumulative (Not B). Based on available data the assessed chemical is categorised as Not Bioaccumulative.

### Toxicity

Toxic (T). Based on available ecotoxicity values below 1 mg/L (acute invertebrates and algae toxicity) the assessed chemical is categorised as Toxic.

## Environmental risk characterisation

Although the assessed chemical is persistent and toxic, it does not meet all three PBT criteria and is hence unlikely to have unpredictable long-term effects (EPHC 2009). A Risk Quotient (PEC/PNEC) for the aquatic compartment was not calculated as the currently available information indicates the assessed chemical will have limited bioavailability and the release to the environment is expected to be minimal. As such, the risk from the assessed chemical can be managed, based on consideration of the environmental hazard characteristics and estimated releases.

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