Australian Government
Department of Health
Australian Industrial Chemicals Introduction Scheme

# Compounds of dimethyltin

## Evaluation statement

**28 January 2022**

**Draft**



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# AICIS evaluation statement

## Subject of the evaluation

Compounds of dimethyltin

## Chemicals in this evaluation

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| 9-Octadecenoic acid, 2-mercaptoethyl ester, (Z)-, reaction products with dichlorodimethylstannane, sodium sulfide ($Na_2S$) and trichloromethylstannane | 68442-12-6 |

## Reason for the evaluation

The Evaluation Selection Analysis indicated a potential risk to human health.

## Parameters of evaluation

The chemicals are a group of dimethyl tin compounds listed on the Australian Inventory of Industrial Chemicals (the Inventory). This evaluation is a human health risk assessment for all identified industrial uses of these chemicals.

These chemicals have been assessed as a group because the toxicity of organotin compounds depends largely on the organotin moiety, and these chemicals are structurally similar. Based on a review of the available information, dimethyltin compounds have been reported to cause reproductive, neurodevelopmental, nervous system and immune system toxicity. These human health effects are likely to be the main drivers of any risk management recommendations for this group of chemicals.

In this evaluation, CAS No. 51287-84-4 will be referred to as dimethyltin bis(dodecylmercaptide).

## Summary of evaluation

### Summary of introduction, use and end use

There is currently no specific information about the use or volume of use of these chemicals in Australia. Data on emissions and sources of emissions for organotin compounds in Australia indicate site limited use in glass and glass product manufacturing and polymer product manufacturing.

Based on international information, dimethyltin bis(dodecylmercaptide) is used as a catalyst and process regulator in the manufacture of plastic and other products used in a wide range of commercial applications. No information is available for the chemical CAS No. 68442-12-

6, but it is expected to have site limited uses similar to other dimethyltin compounds (refer to **Supporting information** section).

## Human health

### Summary of health hazards

There is limited toxicological information for dimethyltin bis(dodecylmercaptide) and none for the chemical CAS No. 68442-12-6. The main driver for the toxicity of dimethyltin compounds is expected to be the dimethyltin moiety. Therefore, available data for other dimethyltin compounds, including dimethyltin dichloride (DMTC) and dimethyltin mercaptoacetate compounds, are used to draw conclusions regarding the systemic effects of chemicals in this group. These dimethyltin compounds were assessed previously and their reports should be read in conjunction with this Evaluation Statement (NICNAS 2018a; NICNAS 2018b).

Based on read across, the critical health effects for risk characterisation are adverse systemic long term effects on:

- reproduction and neurodevelopment
- the immune and nervous systems.

Exposure to DMTC has been linked to decreased thymus weights in males, thymus atrophy in both sexes and increased kidney weights in females with histopathological changes in the thymus, brain and kidneys in both sexes. Neurotoxic effects were noted with signs including convulsions and tremors. Histopathological changes included neuronal necrosis, ventricular dilation, and white matter vacuolisation in the brain and spinal cords (NICNAS 2018a). The available data on reproductive toxicity for DMTC indicated the presence of foetal variations and malformations, and developmental neurotoxicity at low doses in some of the animal studies (NICNAS 2018a).

Based on the available data for DMTC (NICNAS 2018a) and dimethyltin bis(2-ethylhexyl mercaptoacetate (DMT(2-EHMA)) (NICNAS 2018b), the chemicals are not considered to be genotoxic. Carcinogenicity was not observed in long term studies using mixtures of mono- and dimethyltin compounds (WHO 2006).

Based on limited information for dimethyltin bis(dodecylmercaptide) and read across data from dimethyltin mercaptoacetate compounds, the chemicals may have low to moderate acute oral and inhalation toxicity and low acute dermal toxicity.

Experimental, read across and in silico data indicate that the chemicals in this group are not expected to be irritating to the skin or eyes. This is supported by QSAR modelling for dimethyltin bis(dodecylmercaptide).

There are no data on skin sensitisation. Although dimethyltin dimercaptoacetate compounds are skin sensitisers (NICNAS 2018b), the anionic ligand may contribute to this effect. No structural alerts for protein binding based on the mechanistic profiling functionality were found for dimethyltin bis(dodecylmercaptide) using OECD QSAR Toolbox v4.2.

### Health hazard classification

These chemicals satisfy the criteria for classification according to the Globally Harmonized System of Classification and Labelling of Chemicals (GHS) for hazard classes relevant for work health and safety. This evaluation does not consider classification of physical and

environmental hazards. These recommended classifications are based on read across principles (see **Supporting Information – Grouping Rationale** section). If empirical data become available for either member of the group indicating that a lower (or higher) classification is appropriate for a specific chemical, this data may be used to amend the default classification for that chemical.

| Health hazards | Hazard category | Hazard statement |
|---|---|---|
| Specific target organ toxicity - repeated dose exposure | STOT Rep. Exp. 1 | H372: Causes damage to the nervous system and immune system through prolonged or repeated exposure |
| Reproductive toxicity | Repr. 2 | H361d: Suspected of damaging the unborn child |

### Summary of health risk

**Public**

These chemicals are currently listed on in the Poisons Standard–the Standard for the Uniform Scheduling of Medicines and Poisons (the SUSMP), Schedule 7 for tin organic compounds. At concentrations greater than 1%, these chemicals are not available to the general public. A number of warning statements, first aid instructions and safety directions relating to tin organic compounds may apply (TGA 2021).

Based on the available use information, the public may be exposed to the chemicals at very low concentrations in articles through their use in the manufacture of plastics and potential use in food contact applications.

Internationally, a group tolerable daily intake (TDI) of (0.1 µg/kg bw as Sn) for organotin compounds in foodstuffs, based on systemic effects, has been established (European Commission 2009).

To reduce the identified risk of organotin compounds transferred from food packaging to foodstuffs, the overall exposure should be lower than the TDI. The dominant contribution to human intake of organotin compounds (mainly tributyltin) is via consumption of fish. Exposure to other organotin compounds, including these chemicals, is expected to be generally low both from food contact and handling plastic articles.

Based on the available use information, there are no identified risks to the public that require further risk management.

**Workers**

During product formulation and packaging, dermal and inhalation exposure might occur, particularly where manual or open processes are used. These could include transfer and blending activities, quality control analysis, and cleaning and maintaining equipment. Worker exposure to the chemical at lower concentrations could also occur while using formulated products containing the chemical. The level and route of exposure will vary depending on the method of application and work practices employed. Good hygiene practices to minimise incidental oral exposure are expected to be in place.

Given the critical systemic long term health effects, these chemicals could pose a risk to workers.

Control measures to minimise dermal exposure and inhalation exposure (if aerosolised) are needed to manage the risk to workers (see **Proposed means for managing any risks** section).

Control measures implemented due to the reprotoxicity and repeated dose classifications are expected to be sufficient to protect workers from any potential sensitisation health effects.

# Proposed 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.

### 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.

Control measures that could be implemented to manage the risk arising from dermal and inhalation exposure to these chemicals include, but are not limited to:

- using closed systems or isolating operations
- minimising manual processes and work tasks through automating processes
- adopting work procedures that minimise splashes and spills
- cleaning equipment and work areas regularly
- using protective equipment that is designed, constructed, and operated to ensure that the worker does not come into contact with these chemicals.

Measures required to eliminate or manage risk arising from storing, handling and using these hazardous chemicals depend on the physical form and how these chemicals are used.

These control measures may need to be supplemented with:

- conducting health monitoring for any worker who is at significant risk of exposure to these chemicals if valid techniques are available to monitor the effect on the worker's health
- conducting air monitoring to ensure control measures in place continue to work effectively.

Personal protective equipment should not solely be relied upon to control risk and should only be used when all other reasonably practicable control measures do not eliminate or sufficiently minimise risk.

Model codes of practice, available from the Safe Work Australia website, provide information on how to manage the risks of hazardous chemicals in the workplace, prepare an SDS and label containers of hazardous chemicals. Your Work Health and Safety regulator should be contacted for information on Work Health and Safety laws and relevant Codes of Practice in your jurisdiction.

## Conclusions

The conclusions of this evaluation are based on the information described in this Evaluation Statement.

Considering the proposed means of managing risks, the Executive Director is satisfied that the identified human health risks can be managed within existing risk management frameworks. This is provided that all requirements are met under environmental, workplace health and safety and poisons legislation as adopted by the relevant state or territory and the proposed means of managing the risks identified during this evaluation are implemented.

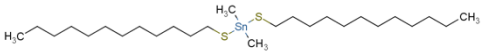
Note: Obligations to report additional information about hazards under *Section 100 of the Industrial Chemicals Act 2019* apply.

# Supporting information

## Grouping rationale

This group of chemicals consists of dimethyltin bis(dodecylmercaptide) and a UVCB, CAS No. 68442-12-6. Both compounds are expected to release dimethyltin compounds following metabolism, although toxicokinetic data is limited to one in chemico hydrolysis study for the former chemical. Di-substituted organotin compounds have the general formula $R_2SnX_2$. The toxicity of organotin compounds depends largely on the organotin moiety (R group), with the anionic ligand (X) mostly influencing physicochemical properties and local toxicity. Although CAS No. 68442-12-6 may also release monomethyltin compounds, the toxicity of monoalkyltin compounds is lower than that of the related dialkyltin compounds.

## Chemical identity

| | |
|---|---|
| Chemical name | Stannane, bis(dodecylthio)dimethyl- |
| CAS No. | 51287-84-4 |
| Synonyms | dimethyltin bis[n-dodecylmercaptide]<br>dimethyltin bis(lauryl mercaptide) |
| Structural formula |  |
| Molecular formula | C26H56S2Sn |
| Molecular weight (g/mol) | 551.57 |
| SMILES | S(CCCCCCCCCCCC)[Sn](SCCCCCCCCCCCC)(C)C |
| Chemical description | Organometallic compound |

| | |
|---|---|
| Chemical name | 9-Octadecenoic acid, 2-mercaptoethyl ester, (Z)-, reaction products with dichlorodimethylstannane, sodium sulfide ($Na_2S$) and trichloromethylstannane |
| CAS No. | 68442-12-6 |
| Synonyms | - |
| Structural formula | No structure available |
| Molecular formula | Not specified |
| Molecular weight (g/mol) | Not specified |

| | |
|---|---|
| SMILES | Not specified |
| Chemical description | Organometallic compound and UVCB |

# Relevant physical and chemical properties

Dimethyltin bis(dodecylmercaptide) is an extremely pale liquid with the following properties:

- boiling point (predicted) 532.2±33.0 °C at 760 Torr (mmHg)
- vapour pressure (predicted) 0.0 +/- 1.4 mm Hg at 25ºC
- density (experimental) 1.08 g/cm$^3$.

Based on the predicted vapour pressure, this chemical has low volatility.

There is no information on the physical or chemical properties for CAS No. 68442-12-6.

# Introduction and use

## Australia

No specific information is available regarding the introduction, import and use of these chemicals in Australia.

The National Pollutant Inventory (NPI) provides information on emission sources of organotin compounds in Australia. The following site limited sources were identified by the NPI in 2019/2020:

- glass and glass product manufacturing
- polymer product manufacturing.

## International

The following international uses for dimethyltin bis(dodecylmercaptide) have been identified through the:

- European Union Registration, Evaluation and Authorisation of Chemicals (REACH)
- Substances in Preparations in Nordic countries (SPIN) database.

Based on international use information, the chemical is reported to be used in site limited applications as a catalyst, process regulator and heat stabiliser in the manufacture of plastic products. It is also used for the manufacture of textile, leather or fur, wood and wood products, pulp, paper and paper products, chemicals, rubber products, fabricated metal products, electrical, electronic and optical equipment, machinery and vehicles and furniture.

These products may have a number of commercial applications including:

- adhesives and sealants
- insulating materials
- construction materials
- coating products
- metal surface treatment products
- non-metal-surface treatment products
- paper chemicals
- textile treatment products and dyes.

Some of these commercial uses may also be used in domestic applications. No consumer uses are registered under REACH and the SPIN database suggests that the registered product uses do not indicate direct exposure to consumers.

No specific information is available for CAS No. 68442-12-6. The chemical was reported under the US Chemical Data Reporting (CDR) under the *Toxic Substances Control Act (US EPA 2012; US EPA 2016)* but no uses were identified. In general, dimethyltin compounds are used in the manufacture of plastics or other products.

# Existing Australian regulatory controls

## AICIS

No specific controls are currently available for these chemicals.

## Public

Tin organic compounds are listed in the Poisons Standard—SUSMP in Schedule 7 (TGA, 2021). This entry covers the chemicals in this group.

"TIN ORGANIC COMPOUNDS, being dialkyl, trialkyl and triphenyl tin compounds where the alkyl group is methyl, ethyl, propyl or butyl except:

a) when separately specified in this Schedule;

b) in plastics;

c) in semi-solid sealants, adhesives or elastomers containing 1% or less of the dialkyl, trialkyl or triphenyl tin component; or

d) in paint containing 1% or less of such compounds calculated as tin in the non-volatile content of the paint."

Schedule 7 chemicals are described as: 'Dangerous poisons – Substances with a high potential for causing harm at low exposure and which require special precautions during manufacture, handling or use. These poisons should be available only to specialised or authorised users who have the skills necessary to handle them safely. Special regulations restricting their availability, possession, storage or use may apply.' (TGA 2021).

### Workers

Tin and its compounds are listed in the Work Health and Safety Regulations (2021 revision) as restricted hazardous chemicals—the restricted use is 'abrasive blasting at a concentration of greater than 0.1% as tin' (SWA 2021).

These chemicals are not specifically listed as hazardous chemicals on the Hazardous Chemicals Information system (HCIS) (SWA).

Tin organic compounds (as Sn) have an exposure standard of 0.1 mg/m$^3$ time weighted average (TWA) and 0.2 mg/m$^3$ short term exposure limit (STEL) (SWA).

In 2020, Safe Work Australia reviewed and recommended to retain the TWA. The recommended TWA is considered protective for effects on the central nervous system and other systems. A STEL was not recommended due to insufficient data relating to acute exposures (SWA 2020). At the time of publication of this Evaluation Statement, these workplace exposure standards were yet to be finalised.

## International regulatory status

### Exposure standards

The following exposure standards were identified for tin, organic compounds (as Sn) (Chemwatch):

An exposure limit of 0.1 mg/m$^3$ TWA and 0.2–0.4 mg/m$^3$ STEL in different countries such as Bulgaria, Canada (Alberta, British Columbia, Ontario, Quebec, Saskatchewan, Yukon), Denmark, Egypt, Estonia, France, Greece, Malaysia, Mexico, Norway, Philippines, Singapore, South Africa, Spain, Sweden, Taiwan, the United Kingdom and the United States of American (California, Hawaii, Minnesota, Tennessee, Vermont, Washington).

### European Union

Tin compounds (organic) are listed on the following (Chemwatch):

- Council of Europe Resolution AP (92) 2 on control of aids to polymerisation for plastic materials and articles intended to come into contact with foodstuffs—Limits for finished articles; a limit of 0.05 mg/kg (as Sn) applies.

## Health hazard information

### Toxicokinetics

Studies have shown that in general, sulfur or carboxylate-based ligands of organotin compounds are easily displaced under mild physiological conditions (NICNAS, 2018b). Abiotic hydrolysis of dimethyltin bis(dodecylmercaptide) has been studied. However, no data are available regarding the in vivo metabolism of these chemicals.

The hydrolysis of dimethyltin bis(dodecylmercaptide) was studied using Organisation for Economic Co-operation and Development (OECD) Test Guideline (TG) 111 at pH 1.2, 4, 7 and 9 using NMR spectroscopy. The chemical was reported to be hydrolytically stable at pH

4, 7 and 9. After 5 days of hydrolysis at 50 °C, less than 10% of the test material was hydrolysed (half-life at 25 °C >1 year). At simulated gastric conditions (0.1 M HCl/pH 1.2 at 37 °C/4 h) the only identifiable breakdown product was the monochloride substituted product of the test material, chlorododecylthiodimethylstannane (REACH).

## Acute toxicity

### Oral

Limited data are available. Dimethyltin bis(dodecylmercaptide) has a reported lethal dose (LD50) in rats of 8500 mg/kg bw (no study details) indicating low acute oral toxicity. Sub-lethal signs of toxicity included general depressed activity, somnolence and haemorrhage (CCOHS).

Dimethyltin alkyl mercaptoacetate compounds have moderate oral acute toxicity with median LD50 values in the range 1000–1735 mg/kg bw (NICNAS 2018b).

### Dermal

No data are available for these chemicals. Dimethyltin alkyl mercaptoacetate compounds have low acute dermal toxicity (NICNAS 2018b).

### Inhalation

Based on the limited data, dimethyltin bis(dodecylmercaptide) has moderate acute inhalation toxicity. An Low C50 in rats of 3.3 mg/L was reported with no study details. Sub-lethal signs of toxicity included unspecified effects on the lungs and thorax in addition to haemorrhage (CCOHS).

Dimethyltin alkyl mercaptoacetate compounds have low acute inhalation toxicity (NICNAS 2018b).

Given the limited study details for the lethal concentration (LC50 value), classification is not warranted.

## Corrosion/Irritation

### Skin irritation

Based on two in vitro studies, dimethyltin bis(dodecylmercaptide) is not expected to be irritating to the skin.

In a GLP compliant in vitro skin corrosion assay conducted in accordance with OECD TG 431, the chemical was applied to reconstructed human epidermis (EpiDerm human skin model) for 3 and 60 minutes. The mean tissue viability was 80.9 % and 82.3% after 3 and 60 minutes respectively. Substances that do not reduce viability to less than 50% after 3 minutes and less than 15% after 60 minutes using this human skin model are classified as non-corrosive. Therefore, the chemical is considered to be unlikely to have the potential to cause corrosion in vivo following application to skin (REACH).

In a GLP compliant in vitro skin irritation study conducted in accordance with OECD TG 439 (in vitro reconstructed human epidermis (RHE) test method for skin irritation), the chemical

was applied to RhE for an exposure period of 15 minutes followed by an observation period of 42 hours. A mean tissue viability value of 80.9% was reported for the chemical in this study, and it was determined not to be irritating to the skin (test chemicals may be considered to be non-irritating to skin if the tissue viability after exposure and post-treatment incubation is >50%). Interpretation of results obtained from OECD TG 439 studies do not allow for distinction between irritation and corrosion (REACH).

The corrosive effects observed for DMTC (NICNAS, 2018a) are not expected to occur for these chemicals. Dimethyltin alkyl mercaptoacetate compounds are considered to be slight skin irritants (NICNAS 2018b).

### Eye irritation

Based on one in vitro study, dimethyltin bis(dodecylmercaptide) is not expected to be irritating to eyes.

In a GLP compliant ex vivo eye corrosivity/irritation study conducted according to OECD TG 437, the chemical was applied to 3 bovine corneae per experiment. The mean in vitro irritancy score (IVIS) was 0.7 (IVIS >55 is regarded as serious eye damage and IVIS $\leq$3 is UN GHS No Category). Based on the criteria of the assay, the chemical did not meet the GHS criteria for classification (REACH).

The corrosive effects observed for DMTC (NICNAS 2018a) are not expected to occur for these chemicals. Dimethyltin alkyl mercaptoacetate compounds are considered to be slight eye irritants (NICNAS 2018b).

# References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