



**Australian Government**

**Department of Health**

Australian Industrial Chemicals Introduction Scheme

# **2-Thiopheneethanol, tetrahydro-2-methyl-5-(1-methylethyl)-**

**Assessment statement (CA09314)**

**6 February 2021**

Final



## Table of contents

AICIS Assessment Statement.....	1
Chemical in this Assessment.....	1
Reason for the Assessment.....	1
Defined Scope of Assessment.....	1
Summary of Assessment.....	1
Conclusions.....	3
Recommendations.....	3
Supporting Information.....	4
Chemical Identity.....	4
Relevant Physical and Chemical Properties.....	4
Human Exposure.....	5
Health Hazard Information.....	5
Environmental Exposure.....	6
Environmental Effects.....	7
Categorisation of Environmental Hazard.....	7
Environmental Risk Characterisation.....	7
References.....	8

# AICIS Assessment Statement

## Chemical in this Assessment

Name	CAS Registry Number
2-Thiopheneethanol, tetrahydro-2-methyl-5-(1-methylethyl)-	1612888-42-2

## Reason for the Assessment

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

### Certificate Application Type

**Very low to low risk**

Based on introduction, use and end use information described in the application, the human health and environment exposure bands of the introduction are 3 and 2 respectively [item 5 clause 1 and item 2 clause 3 of Schedule 1, *Industrial Chemicals (General) Rules 2019* (the Rules)]. The assessed chemical does not have any of the hazard characteristics in human health hazard band C and environment hazard band D. In accordance with table item 10 section 28 and table item 12 section 29 of the Rules, the indicative human health and environment risk for the proposed introduction are both in the low risk category.

## Defined Scope of Assessment

The chemical has been assessed:

- as imported into Australia  $\leq 1$  tonne/annum
- as a component of liquid fragrance blend at  $\leq 0.1\%$  concentration for reformulation of end use cosmetic and household products, and
- as a component of end use cosmetic and household products at  $\leq 0.01\%$  concentration.

## Summary of Assessment

### Summary of Introduction, Use and End Use

The assessed chemical will be imported into Australia as a component of a liquid fragrance blend formulation at  $\leq 0.1\%$  concentration for reformulation into cosmetic and household products, or as a component of end use cosmetic and household products at  $\leq 0.01\%$  concentration. End-use products containing the assessed chemical at  $\leq 0.01\%$  concentration will be widely used by consumers as well as workers in beauty and hairdressing salons, and cleaners.

## Human Health

### Summary of health hazards

Only limited hazard information is available on the assessed chemical. The hazard profile of the assessed chemical cannot be fully determined at the time of the assessment. The assessed chemical is not listed on the **list of chemicals with high hazards for categorization** (Appendix 8.1 of the AICIS *Industrial Chemicals Categorisation Guidelines*) when checked at the time of this assessment for carcinogenicity, reproductive toxicity, developmental toxicity, adverse effects mediated by an endocrine mode of action and genetic toxicity. There is no available evidence to demonstrate that the assessed chemical has any of the hazard characteristics in human health hazard band C.

### Health Hazard Classification

As only limited toxicology data were provided, the assessed chemical cannot be classified for hazard classes relevant for work health and safety, according to the *Globally Harmonised System of Classification and Labelling of Chemicals* (GHS, United Nations 2017), as adopted for industrial chemicals in Australia.

However, based on evidence from structurally similar chemicals, the applicant provided the following classifications for the assessed chemical in relation to human health:

Human Health Hazard	Hazard Category	Hazard Statement
Acute toxicity – oral	Category 4	H302: Harmful if swallowed
Skin irritation	Category 2	H315: Causes skin irritation
Eye irritation	Category 2	H319: Causes serious eye irritation

The assessed chemical will not be introduced into Australia at concentrations that warrant the above hazard classifications.

### Summary of Health Risk

#### Public

Based on the available information the assessed chemical is expected to have low risk potential when used at low end use concentration of  $\leq 0.01\%$ . There are no identified risks to the public health that require specific risk management measures, if the assessed chemical is introduced and used in accordance with the terms of the certificate.

#### Workers

When introduced at  $\leq 0.1\%$  concentration for reformulation and at  $\leq 0.01\%$  concentration for end use as a fragrance component in accordance with the terms of the certificate, the assessed chemical is unlikely to pose a risk to workers.

## Environment

### Summary of Environmental Hazards

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

- persistent (P) based on ready biodegradability data
- not Bioaccumulative (not B) based on the octanol-water partition coefficient
- not Toxic (not T) based on ecotoxicity data for fish

### Environmental Hazard Classification

The assessed chemical is formally classified under the GHS for acute and chronic toxicities as H412: Harmful to aquatic life with long lasting effects based on the ecotoxicological endpoint and biodegradability data.

Environmental Hazard	Hazard Category	Hazard Statement
Chronic Aquatic	Category 3	H412: Harmful to aquatic life with long lasting effects

### Summary of Environmental Risk

Based on the end use as a fragrance, the majority of the assessed chemical is expected to be released into sewage treatment plants (STPs). The calculated environmental risk quotient for the assessed use of the chemical is  $\leq 0.01$ .

Therefore, there are no identified risks to the environment that require specific risk management measures, if the assessed chemical is introduced in accordance with the terms of the certificate.

## Conclusions

The Executive Director is satisfied that when the assessed chemical is introduced in accordance with the terms of the assessment certificate the human health and environment risks can be managed. 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.

## Recommendations

No specific recommendations for safe use of the assessed chemical are required when the chemical is introduced in accordance with the terms of the certificate.

# Supporting Information

## Chemical Identity

The assessed chemical has a degree of purity > 90%. It contains 2 diastereomers in an approximately 1:1 ratio, individually identified as follows:

CAS Number	2089680-80-6
Chemical Name	2-Thiopheneethanol, tetrahydro-2-methyl-5-(1-methylethyl)-, (2 <i>R</i> ,5 <i>S</i> )- <i>rel</i> -

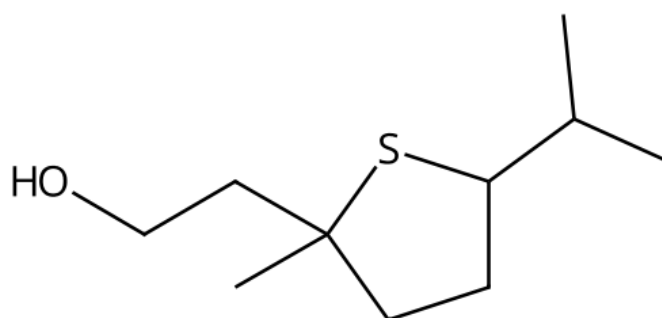
CAS Number	2089680-79-3
Chemical Name	2-Thiopheneethanol, tetrahydro-2-methyl-5-(1-methylethyl)-, (2 <i>R</i> ,5 <i>R</i> )- <i>rel</i> -

## Other Chemical Identity Information

Synonyms

2-[2-methyl-5-(propan-2-yl)tetrahydrothiophen-2-yl]ethanol (IUPAC name)  
Lemon Sulfur Alcohol (trade name)  
Pyromist (trade name)

Structural Formula



Molecular Formula

C<sub>10</sub>H<sub>20</sub>S

Molecular Weight (g/mol)

188.33

SMILES

CC1(CCO)CCC(S1)C(C)C

## Relevant Physical and Chemical Properties

Physical Form

Colourless liquid

Melting Point

Not determined, the chemical is liquid at room temperature

Boiling Point

263.8 °C

Vapour Pressure	0.34 Pa at 24 °C
Water Solubility	2363 mg/L at 24 °C
Flash Point	Not determined, SDS of the chemical reported a flash point of 88 °C
Hydrolysis as a function of pH	Does not contain functional groups which hydrolyse under environmental pH (4-9)
Ionisable in the Environment?	No
pKa	N/A
log Kow	3.46
log Koc	2.19

The assessed chemical will only be imported into Australia at concentration  $\leq 0.1\%$ .

## Human Exposure

### Workers

#### Reformulation

During reformulation operations, dermal and ocular exposure of workers to the assessed chemical at  $\leq 0.1\%$  concentration is possible when weighing and transferring the fragrance blends containing the chemical from the import containers into blending equipment and quality control testing.

#### Professional End Use

Professional cleaners and beauty salon workers may come into contact with the assessed chemical at up to 0.01% concentration when using the cleaning and cosmetic end use products containing the chemical. Depending on the method of application, dermal and accidental ocular exposure may occur when applying the products using brush, spray, sponge or cloth.

### Public

There will be widespread and repeated exposure of the public to the assessed chemical at  $\leq 0.01\%$  concentration through the use of a wide range of cosmetic and household products. The primary route of exposure will be dermal, while ocular and inhalation exposures are also possible, particularly if the products are applied on face and by spray. Oral exposure may also occur with the use of oral-care products containing the assessed chemical.

## Health Hazard Information

The assessed chemical has a molecular weight of 188 g/mol and is highly water soluble. Therefore, it could be readily absorbed through biological membranes when exposed.

No toxicology data for the assessed chemical was provided, except for an *in vitro* genetic toxicity study. The assessed chemical was found to be non-mutagenic in the *in vitro* bacterial reverse mutation (Ames) test conducted according to the OECD TG471.

The application dossier contains hazard information for the assessed chemical, which indicates the chemical is harmful if swallowed and causes skin irritation and serious eye irritation, based on evidence from structurally similar chemicals and computer modelling.

## Environmental Exposure

The assessed chemical is not expected to be released into the environment during reformulation, transport or storage. Based on the assessed use as a fragrance in various consumer products, the majority of the assessed chemical is expected to be released to sewers.

## Environmental Fate

The assessed chemical is readily soluble in water, moderately lipophilic and expected to have medium mobility in soil based on the measured endpoints conducted according to OECD test guidelines. The chemical is not readily biodegradable (7% degradation over 28 days in OECD TG 301F study) and does not contain any functional groups susceptible to hydrolysis or dissociation under environmental pH range (pH 4 – 9). A majority proportion of the chemical will be disposed of into STPs and released to environment with effluent from STPs. The chemical is not expected to bioaccumulate in the environment based on its estimated low octanol-water partition coefficient ( $\log K_{ow} = 3.46$ ).

## Predicted Environmental Concentration (PEC)

The predicted environmental concentrations (PEC) in water (receiving environments) have been calculated based on 100% release of the assessed chemical (from the introduction volume) into sewer systems nationwide over 365 days per annum. The extent to which the assessed chemical is removed from the effluent in STP processes is based on its physico-chemical properties and its limited biodegradability, modelled by SimpleTreat 3.0 (Struijs, 1996) and is estimated to be 4%. Therefore 96% of the total introduction volume is estimated to be released to the aquatic environment. The calculation of the PEC is detailed in the table below:

Total Annual Import Volume	1000	kg/year
Proportion expected to be released to sewer	100%	
Annual quantity of chemical released to sewer	1000	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	24.386	million
Removal within STP	4%	mitigation



Daily effluent production	4877	ML
Dilution Factor - River	1.0	
Dilution Factor - Ocean	10.0	
PEC - River	0.54	µg/L
PEC - Ocean	0.054	µg/L

## Environmental Effects

### Effects on Aquatic Life

#### Acute toxicity

Based on the ecotoxicological endpoint provided by the applicant, the assessed chemical is harmful to fish (96 h LC50 = 43.8 mg/L).

#### Predicted No-Effect Concentration (PNEC)

A Predicted No-Effect Concentration (PNEC) was calculated based on the above acute endpoint for fish using an assessment factor of 1000 as only one acute trophic endpoint is available. The resulting PNEC is 43.8 µg/L.

## Categorisation of Environmental Hazard

The categorisation of the environmental hazards of the assessed chemical according to domestic environmental hazard thresholds is presented below:

#### Persistence

Persistent (P). Based on ready biodegradability study (not readily biodegradable after 28 days), the assessed chemical is categorised as Persistent.

#### Bioaccumulation

Not Bioaccumulative (Not B). Based on the measured log Kow value (log Kow < 4.2), the assessed chemical is categorised as Not Bioaccumulative.

#### Toxicity

Not Toxic (Not T). Based on the available ecotoxicity value above 1 mg/L, the assessed chemical is categorised as Not Toxic.

## Environmental Risk Characterisation

The risk quotient (RQ = PEC/PNEC) for the assessed chemical is calculated to be 0.01 for riverine compartments and < 0.01 for oceanic compartments. Therefore, the assessed

chemical is unlikely to pose significant risk to aquatic life based on its low hazard characteristics and proposed introduction and use pattern.

## References

Struijs J (1996). SimpleTreat 3.0: a model to predict the distribution and elimination of chemicals by sewage treatment plants. National Institute of Public Health and the Environment, Bilthoven, The Netherlands.

United Nations (2017) [Globally Harmonised System of Classification and Labelling of Chemicals \(GHS\), 7th Revised Edition](#). United Nations Economic Commission for Europe, Geneva, Switzerland.

