

according to Regulation (EC) No. 1907/2006

Creation Date 07-Jun-2010 Revision Date 07-Feb-2024 Revision Number 3

# SECTION 1: IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

#### 1.1. Product identifier

Product Description: 4-(Methylthio)benzeneboronic acid

Cat No. : L14572

Synonyms 4-Thioanisoleboronic acid

**CAS No** 98546-51-1 **Molecular Formula** C7 H9 B O2 S

REACH registration number -

#### 1.2. Relevant identified uses of the substance or mixture and uses advised against

Recommended Use Laboratory chemicals.
Uses advised against No Information available

## 1.3. Details of the supplier of the safety data sheet

Company

Thermo Fisher (Kandel) GmbH

Erlenbachweg 2, 76870 Kandel, Germany

Tel: +49 (0) 721 84007 280 Fax: +49 (0) 721 84007 300

Swiss distributor - Fisher Scientific AG Neuhofstrasse 11. CH 4153 Reinach

Tel: +41 (0) 56 618 41 11

https://www.fishersci.ch/ch/en/customer-help-

support/forms/email-us.html

E-mail address begel.sdsdesk@thermofisher.com

## 1.4. Emergency telephone number

For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11 Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99 **CHEMTREC** Tel. No.**US**:001-800-424-9300 / **Europe**:001-703-527-3887

customers in Switzerland:

Tox Info Suisse Emergency Number: 145 (24hr)

Tox Info Suisse: +41-44 251 51 51 (Emergency number from abroad)

Chemtrec (24h) Toll-Free: 0800 564 402 Chemtrec Local: +41-43 508 20 11 (Zurich)

## **SECTION 2: HAZARDS IDENTIFICATION**

## 2.1. Classification of the substance or mixture

ALFAAL14572

#### 4-(Methylthio)benzeneboronic acid

Revision Date 07-Feb-2024

#### CLP Classification - Regulation (EC) No 1272/2008

#### **Physical hazards**

Based on available data, the classification criteria are not met

#### **Health hazards**

Skin Corrosion/Irritation

Serious Eye Damage/Eye Irritation

Specific target organ toxicity - (single exposure)

Category 2 (H315)

Category 2 (H319)

Category 3 (H335)

#### **Environmental hazards**

Based on available data, the classification criteria are not met

Full text of Hazard Statements: see section 16

#### 2.2. Label elements



#### Signal Word

#### Warning

## **Hazard Statements**

H319 - Causes serious eye irritation

H335 - May cause respiratory irritation

H315 - Causes skin irritation

## **Precautionary Statements**

P302 + P352 - IF ON SKIN: Wash with plenty of soap and water

P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing

P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing

P312 - Call a POISON CENTER or doctor if you feel unwell

P280 - Wear protective gloves/protective clothing/eye protection/face protection

## 2.3. Other hazards

This product does not contain any known or suspected endocrine disruptors

## **SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS**

#### 3.1. Substances

	Component	CAS No	EC No	Weight %	CLP Classification - Regulation (EC) No 1272/2008
I	Boronic acid, B-[4-(methylthio)phenyl]-	98546-51-1		>95	STOT SE 3 (H335)
-					Skin Irrit. 2 (H315)
-					Eye Irrit. 2 (H319)

## **REACH** registration number

Full text of Hazard Statements: see section 16

## **SECTION 4: FIRST AID MEASURES**

#### 4.1. Description of first aid measures

**General Advice** If symptoms persist, call a physician.

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get **Eve Contact** 

medical attention.

**Skin Contact** Wash off immediately with plenty of water for at least 15 minutes. Get medical attention.

Ingestion Clean mouth with water and drink afterwards plenty of water. Get medical attention if

symptoms occur.

Remove to fresh air. If breathing is difficult, give oxygen. Get medical attention. Inhalation

Self-Protection of the First Aider Use personal protective equipment as required.

#### 4.2. Most important symptoms and effects, both acute and delayed

None reasonably foreseeable.

#### 4.3. Indication of any immediate medical attention and special treatment needed

Notes to Physician Treat symptomatically.

#### **SECTION 5: FIREFIGHTING MEASURES**

## 5.1. Extinguishing media

#### **Suitable Extinguishing Media**

Water spray, carbon dioxide (CO2), dry chemical, alcohol-resistant foam.

## Extinguishing media which must not be used for safety reasons

No information available.

## 5.2. Special hazards arising from the substance or mixture

Thermal decomposition can lead to release of irritating gases and vapors.

## **Hazardous Combustion Products**

Carbon monoxide (CO), Carbon dioxide (CO2), Sulfur oxides.

## 5.3. Advice for firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

## **SECTION 6: ACCIDENTAL RELEASE MEASURES**

## 6.1. Personal precautions, protective equipment and emergency procedures

Ensure adequate ventilation. Use personal protective equipment as required. Avoid dust formation.

Revision Date 07-Feb-2024

#### 4-(Methylthio)benzeneboronic acid

#### 6.2. Environmental precautions

Should not be released into the environment. See Section 12 for additional Ecological Information.

## 6.3. Methods and material for containment and cleaning up

Sweep up and shovel into suitable containers for disposal. Keep in suitable, closed containers for disposal.

#### 6.4. Reference to other sections

Refer to protective measures listed in Sections 8 and 13.

## **SECTION 7: HANDLING AND STORAGE**

#### 7.1. Precautions for safe handling

Wear personal protective equipment/face protection. Ensure adequate ventilation. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation. Avoid dust formation.

## **Hygiene Measures**

Handle in accordance with good industrial hygiene and safety practice.

#### 7.2. Conditions for safe storage, including any incompatibilities

Keep containers tightly closed in a dry, cool and well-ventilated place. To maintain product quality: Keep refrigerated.

Technical Rules for Hazardous Substances (TRGS) 510

Storage Class (LGK) (Germany)

Storage Class/LGK 11

Switzerland - Storage of hazardous substances

Storage class - SC 11/13 https://www.kvu.ch/de/themen/stoffe-und-produkte https://www.kvu.ch/fr/themes/substances-et-produits https://www.kvu.ch/it/temi/sostanze-e-prodotti

Revision Date 07-Feb-2024

#### 7.3. Specific end use(s)

Use in laboratories

## **SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION**

## 8.1. Control parameters

#### **Exposure limits**

This product, as supplied, does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies

## **Biological limit values**

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific regulatory bodies

Revision Date 07-Feb-2024

#### 4-(Methylthio)benzeneboronic acid

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents.

MDHS14/3 General methods for sampling and gravimetric analysis of respirable and inhalable dust

## Derived No Effect Level (DNEL) / Derived Minimum Effect Level (DMEL)

No information available

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

No information available.

## 8.2. Exposure controls

#### **Engineering Measures**

Ensure that eyewash stations and safety showers are close to the workstation location. Ensure adequate ventilation, especially in confined areas.

Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source

#### Personal protective equipment

**Eye Protection** Goggles (European standard - EN 166)

Hand Protection Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Natural rubber	See manufacturers	-	EN 374	(minimum requirement)
Butyl rubber	recommendations			
Nitrile rubber				
Neoprene				
PVC				

**Skin and body protection** Long sleeved clothing.

Inspect gloves before use. observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information) gloves are suitable for the task: Chemical compatability, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion. gloves with care avoiding skin contamination.

**Respiratory Protection** No protective equipment is needed under normal use conditions.

Large scale/emergency use Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits

are exceeded or if irritation or other symptoms are experienced **Recommended Filter type:** Particulates filter conforming to EN 143

Small scale/Laboratory use Maintain adequate ventilation Use a NIOSH/MSHA or European Standard EN 149:2001

approved respirator if exposure limits are exceeded or if irritation or other symptoms are

experiencea.

Recommended half mask:- Valve filtering: EN405; or; Half mask: EN140; plus filter, EN

141

**Environmental exposure controls** No information available.

## **SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES**

#### 4-(Methylthio)benzeneboronic acid

Revision Date 07-Feb-2024

Solid

## 9.1. Information on basic physical and chemical properties

**Physical State** Solid

Off-white **Appearance** Odor Odorless

No data available **Odor Threshold** 

210 - 214 °C / 410 - 417.2 °F **Melting Point/Range** 

Softening Point No data available **Boiling Point/Range** No information available

Flammability (liquid) Not applicable

Flammability (solid,gas) No information available **Explosion Limits** No data available

**Flash Point** No information available Method - No information available

**Autoignition Temperature** No data available **Decomposition Temperature** No data available No information available Hq

**Viscosity** Not applicable

Solid No information available **Water Solubility** 

Solubility in other solvents No information available

Partition Coefficient (n-octanol/water)

**Vapor Pressure** No data available No data available **Density / Specific Gravity Bulk Density** No data available

**Vapor Density** Not applicable Solid

Particle characteristics No data available

9.2. Other information

**Molecular Formula** C7 H9 B O2 S **Molecular Weight** 168.02

**Evaporation Rate** Not applicable - Solid

## **SECTION 10: STABILITY AND REACTIVITY**

10.1. Reactivity None known, based on information available

10.2. Chemical stability

Stable under normal conditions.

10.3. Possibility of hazardous reactions

**Hazardous Polymerization** Hazardous polymerization does not occur.

None under normal processing. **Hazardous Reactions** 

10.4. Conditions to avoid

Incompatible products. Excess heat. Avoid dust formation.

10.5. Incompatible materials

Strong oxidizing agents.

10.6. Hazardous decomposition products

Carbon monoxide (CO). Carbon dioxide (CO2). Sulfur oxides.

## **SECTION 11: TOXICOLOGICAL INFORMATION**

11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

Revision Date 07-Feb-2024

**Product Information** 

(a) acute toxicity;

No data available Oral No data available Dermal Inhalation No data available

Category 2 (b) skin corrosion/irritation;

(c) serious eye damage/irritation; Category 2

(d) respiratory or skin sensitization;

Respiratory No data available No data available Skin

(e) germ cell mutagenicity; No data available

(f) carcinogenicity; No data available

There are no known carcinogenic chemicals in this product

No data available (g) reproductive toxicity;

Category 3 (h) STOT-single exposure;

Results / Target organs Respiratory system.

(i) STOT-repeated exposure; No data available

No information available. **Target Organs** 

(j) aspiration hazard; Not applicable

Solid

**Other Adverse Effects** The toxicological properties have not been fully investigated.

Symptoms / effects,both acute and No information available.

delayed

11.2. Information on other hazards

**Endocrine Disrupting Properties** Assess endocrine disrupting properties for human health. This product does not contain any

known or suspected endocrine disruptors.

## **SECTION 12: ECOLOGICAL INFORMATION**

12.1. Toxicity

No information available. **Ecotoxicity effects** 

12.2. Persistence and degradability No information available

4-(Methylthio)benzeneboronic acid

**12.3. Bioaccumulative potential** No information available

12.4. Mobility in soil No information available

12.5. Results of PBT and vPvB

assessment

No data available for assessment.

12.6. Endocrine disrupting

properties

Endocrine Disruptor Information This product does not contain any known or suspected endocrine disruptors

12.7. Other adverse effects

Persistent Organic Pollutant Ozone Depletion Potential This product does not contain any known or suspected substance This product does not contain any known or suspected substance

## **SECTION 13: DISPOSAL CONSIDERATIONS**

13.1. Waste treatment methods

Waste from Residues/Unused

**Products** 

Waste is classified as hazardous. Dispose of in accordance with the European Directives

Revision Date 07-Feb-2024

on waste and hazardous waste. Dispose of in accordance with local regulations.

**Contaminated Packaging** Dispose of this container to hazardous or special waste collection point.

European Waste Catalogue (EWC) According to the European Waste Catalog, Waste Codes are not product specific, but

application specific.

Other Information Waste codes should be assigned by the user based on the application for which the product

was used. Do not empty into drains.

Switzerland - Waste Ordinance Disposal should be in accordance with applicable regional, national and local laws and

regulations. Ordinance on the Avoidance and the Disposal of Waste (Waste Ordinance,

ADWO) SR 814.600

https://www.fedlex.admin.ch/eli/cc/2015/891/en

## **SECTION 14: TRANSPORT INFORMATION**

IMDG/IMO Not regulated

14.1. UN number

14.2. UN proper shipping name

14.3. Transport hazard class(es)

14.4. Packing group

ADR Not regulated

14.1. UN number

14.2. UN proper shipping name

14.3. Transport hazard class(es)

14.4. Packing group

IATA Not regulated

14.1. UN number

14.2. UN proper shipping name

14.3. Transport hazard class(es)

Revision Date 07-Feb-2024

#### 4-(Methylthio)benzeneboronic acid

14.4. Packing group

14.5. Environmental hazards No hazards identified

**14.6. Special precautions for user** No special precautions required.

14.7. Maritime transport in bulk according to IMO instruments

Not applicable, packaged goods

## **SECTION 15: REGULATORY INFORMATION**

#### 15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture

#### **International Inventories**

Europe (EINECS/ELINCS/NLP), China (IECSC), Taiwan (TCSI), Korea (KECL), Japan (ENCS), Japan (ISHL), Canada (DSL/NDSL), Australia (AICS), New Zealand (NZIoC), Philippines (PICCS). US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

L	Component	CAS No	EINECS	ELINCS	NLP	IECSC	TCSI	KECL	ENCS	ISHL
	Boronic acid, B-[4-(methylthio)phenyl]-	98546-51-1	-	-	-	-	X	-	-	-
				·		,				
- 1	Component	CVCNO	TSCA	I TCCAI	wontory	l Dei	NDGI	VICE	NZIAC	

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
Boronic acid, B-[4-(methylthio)phenyl]-	98546-51-1	-	-	1	1	1	-	-

Legend: X - Listed '-' - Not Listed KECL - NIER number or KE number (http://ncis.nier.go.kr/en/main.do)

#### Authorisation/Restrictions according to EU REACH

Component	CAS No	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization	3	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
Boronic acid, B-[4-(methylthio)phenyl]-	98546-51-1	-	-	-

Not applicable

#### Seveso III Directive (2012/18/EC)

Component	CAS No	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements		
Boronic acid, B-[4-(methylthio)phenyl]-	98546-51-1	Not applicable	Not applicable		

Regulation (EC) No 649/2012 of the European Parliament and of the Council of 4 July 2012 concerning the export and import of dangerous chemicals

Not applicable

Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?

Not applicable

Take note of Directive 98/24/EC on the protection of the health and safety of workers from the risks related to chemical agents at work .

## **National Regulations**

#### 4-(Methylthio)benzeneboronic acid

UK - Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment

**WGK Classification** 

Water endangering class = 2 (self classification)

#### **Swiss Regulations**

Article 4 para. 4 of the Ordinance on the protection of young people in the workplace (SR 822.115) and Article 1 lit. f of the EAER regulation on hazardous work and young people (SR 822.115.2).

Take note on Article 13 Maternity Ordinance (SR 822.111.52) with regards expectant and nursing mothers.

#### 15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

## **SECTION 16: OTHER INFORMATION**

#### Full text of H-Statements referred to under sections 2 and 3

H315 - Causes skin irritation

H319 - Causes serious eye irritation H335 - May cause respiratory irritation

#### Legend

CAS - Chemical Abstracts Service

TSCA - United States Toxic Substances Control Act Section 8(b)

Revision Date 07-Feb-2024

Substances/EU List of Notified Chemical Substances

PICCS - Philippines Inventory of Chemicals and Chemical Substances **IECSC** - Chinese Inventory of Existing Chemical Substances

**KECL** - Korean Existing and Evaluated Chemical Substances

EINECS/ELINCS - European Inventory of Existing Commercial Chemical DSL/NDSL - Canadian Domestic Substances List/Non-Domestic Substances List

**ENCS** - Japanese Existing and New Chemical Substances AICS - Australian Inventory of Chemical Substances

NZIoC - New Zealand Inventory of Chemicals

WEL - Workplace Exposure Limit

**ACGIH** - American Conference of Governmental Industrial Hygienists

**DNEL** - Derived No Effect Level

RPE - Respiratory Protective Equipment LC50 - Lethal Concentration 50% NOEC - No Observed Effect Concentration

PBT - Persistent, Bioaccumulative, Toxic

TWA - Time Weighted Average

IARC - International Agency for Research on Cancer

Predicted No Effect Concentration (PNEC)

LD50 - Lethal Dose 50%

EC50 - Effective Concentration 50% POW - Partition coefficient Octanol:Water vPvB - very Persistent, very Bioaccumulative

ADR - European Agreement Concerning the International Carriage of Dangerous Goods by Road

IMO/IMDG - International Maritime Organization/International Maritime Dangerous Goods Code

**OECD** - Organisation for Economic Co-operation and Development

**BCF** - Bioconcentration factor

ICAO/IATA - International Civil Aviation Organization/International Air Transport Association

MARPOL - International Convention for the Prevention of Pollution from Ships

ATE - Acute Toxicity Estimate VOC - (volatile organic compound)

#### Key literature references and sources for data

https://echa.europa.eu/information-on-chemicals

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

#### **Training Advice**

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

Health, Safety and Environmental Department **Prepared By** 

**Creation Date** 07-Jun-2010 **Revision Date** 07-Feb-2024

**Revision Summary** New emergency telephone response service provider.

Revision Date 07-Feb-2024

This safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006. COMMISSION REGULATION (EU) 2020/878 amending Annex II to Regulation (EC) No. 1907/2006

For Switzerland - Compiled in accordance with the technical provisions referred to in Annex 2, Number 3, ChemO (SR 813.11 - Ordinance on Protection against Dangerous Substances and Preparations).

#### **Disclaimer**

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

**End of Safety Data Sheet**