

according to Regulation (EC) No. 1907/2006

Creation Date 30-Jan-2015 Revision Date 11-Feb-2024 Revision Number 3

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

1.1. Product identifier

Product Description: <u>5-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-pyrrolo[2,3-b]pyridine</u>

 Cat No.:
 H50044

 CAS No
 754214-56-7

 Molecular Formula
 C13H17BN2O2

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

CLP Classification - Regulation (EC) No 1272/2008

ALFAAH50044

5-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-pyrrolo[2,3-b]pyridine

Physical hazards

Based on available data, the classification criteria are not met

Health hazards

Acute oral toxicity
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

H302 - Harmful if swallowed

H315 - Causes skin irritation

H319 - Causes serious eye irritation

H335 - May cause respiratory irritation

Precautionary Statements

P301 + P330 + P331 - IF SWALLOWED: rinse mouth. Do NOT induce vomiting

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

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

P337 + P313 - If eye irritation persists: Get medical advice/attention

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

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

P332 + P313 - If skin irritation occurs: Get medical advice/attention

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
7-Azaindole-5-boronic acid, pinacol ester	754214-56-7		>95	Acute Tox. 4 (H302)

5-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-pyrrolo[2,3-b]pyridine

					Skin Irrit. 2 (H315) Eye Irrit. 2 (H319) STOT SE 3 (H335)
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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.

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

medical attention.

Skin Contact Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists,

call a physician.

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

symptoms occur.

Inhalation Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if

symptoms occur.

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).

5.3. Advice for firefighters

5-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-pyrrolo[2,3-b]pyridine

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

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

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.

Technical Rules for Hazardous Substances (TRGS) 510 Storage Class (LGK) (Germany)

Storage Class/LGK 11

Switzerland - Storage of hazardous substances

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 Storage class - SC

11/13

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

Revision Date 11-Feb-2024

Biological limit values

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

Monitoring methods

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.

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 Nitrile rubber Neoprene Natural rubber	Breakthrough time See manufacturers recommendations	Glove thickness	EU standard EN 374	Glove comments (minimum requirement)
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 When workers are facing concentrations above the exposure limit they must use

appropriate certified respirators.

To protect the wearer, respiratory protective equipment must be the correct fit and be used

and maintained properly

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5-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-pyrrolo[2,3-b]pyridine

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 Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure

limits are exceeded or if irritation or other symptoms are experienced.

Recommended half mask:- Particle filtering: EN149:2001 When RPE is used a face piece Fit Test should be conducted

No information available. **Environmental exposure controls**

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

9.1. Information on basic physical and chemical properties

Physical State Solid

Appearance Off-white

No information available Odor

Odor Threshold No data available

Melting Point/Range 244 - 246 °C / 471.2 - 474.8 °F Measured

Softening Point No data available **Boiling Point/Range** Not applicable

Flammability (liquid) Not applicable Solid

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

Flash Point Not applicable Method - No information available

Autoignition Temperature No data available **Decomposition Temperature** No data available Not applicable рΗ

Not applicable Solid Viscosity

Water Solubility No information available Solubility in other solvents No information available

Partition Coefficient (n-octanol/water)

No data available **Vapor Pressure Density / Specific Gravity** No data available **Bulk Density** No data available Not applicable **Vapor Density**

Solid

No data available Particle characteristics

9.2. Other information

C13H17BN2O2 Molecular Formula **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

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5-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-pyrrolo[2,3-b]pyridine

Hazardous Polymerization Hazardous polymerization does not occur.

Hazardous Reactions None under normal processing.

10.4. Conditions to avoid

Incompatible products. Excess heat. Avoid dust formation.

10.5. Incompatible materials

Acids. Oxidizing agent.

10.6. Hazardous decomposition products

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

SECTION 11: TOXICOLOGICAL INFORMATION

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

Product Information

(a) acute toxicity;

Oral Category 4
Dermal No data available
Inhalation No data available

Toxicology data for the components

(b) skin corrosion/irritation; Category 2

(c) serious eye damage/irritation; Category 2

(d) respiratory or skin sensitization;

Respiratory No data available Skin No data available

(e) germ cell mutagenicity; No data available

(f) carcinogenicity; No data available

There are no known carcinogenic chemicals in this product

(g) reproductive toxicity; No data available

(h) STOT-single exposure; Category 3

Results / Target organs Respiratory system.

(i) STOT-repeated exposure; No data available

Target Organs No information available.

(j) aspiration hazard; Not applicable

Solid

Symptoms / effects,both acute and No information available.

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5-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-pyrrolo[2,3-b]pyridine

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

Ecotoxicity effectsContains no substances known to be hazardous to the environment or that are not

degradable in waste water treatment plants.

12.2. Persistence and degradability No information available

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 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

ALFAAH50044

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

<u>IATA</u> Not regulated

14.1. UN number

14.2. UN proper shipping name

14.3. Transport hazard class(es)

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

nonto

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)

Component	CAS No	EINECS	ELINCS	NLP	IECSC	TCSI	KECL	ENCS	ISHL
7-Azaindole-5-boronic acid,	754214-56-7	-	-	-	-	-	-	-	-
pinacol ester									

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
7-Azaindole-5-boronic acid, pinacol ester	754214-56-7	-	-	-	-	-	-	-

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 Not applicable

Component	CAS No	REACH (1907/2006) -	REACH (1907/2006) -	REACH Regulation (EC
		Annex XIV - Substances	Annex XVII - Restrictions	1907/2006) article 59 -
		Subject to Authorization	on Certain Dangerous	Candidate List of
			Substances	Substances of Very High

ALFAAH50044

5-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-pyrrolo[2,3-b]pyridine

				Concern (SVHC)
7-Azaindole-5-boronic acid, pinacol	754214-56-7	-	-	-
ester				

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
7-Azaindole-5-boronic acid, pinacol ester	754214-56-7	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

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

WGK Classification Water endangering class = 3 (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

H302 - Harmful if swallowed

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)
Inventory

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

Substances List

PICCS - Philippines Inventory of Chemicals and Chemical Substances

ENCS - Japanese Existing and New Chemical Substances

IECSC - Chinese Inventory of Existing Chemical Substances **KECL** - Korean Existing and Evaluated Chemical Substances **NZIOC** - New Zealand Inventory of Chemicals

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ALFAAH50044

Revision Date 11-Feb-2024

TWA - Time Weighted Average

EC50 - Effective Concentration 50%

POW - Partition coefficient Octanol:Water

vPvB - very Persistent, very Bioaccumulative

LD50 - Lethal Dose 50%

Transport Association

ATE - Acute Toxicity Estimate

VOC - (volatile organic compound)

IARC - International Agency for Research on Cancer Predicted No Effect Concentration (PNEC)

ICAO/IATA - International Civil Aviation Organization/International Air

MARPOL - International Convention for the Prevention of Pollution from

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

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

Key literature references and sources for data

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

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

Classification and procedure used to derive the classification for mixtures according to Regulation (EC) 1272/2008 [CLP]:

Ships

Physical hazards On basis of test data **Health Hazards** Calculation method **Environmental hazards** Calculation method

Training Advice

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

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 30-Jan-2015 **Revision Date** 11-Feb-2024

Revision Summary New emergency telephone response service provider.

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

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