

# SAFETY DATA SHEET

Version 6.4  
Revision Date 09/06/2024  
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## SECTION 1: Identification of the substance/mixture and of the company/undertaking

### 1.1 Product identifiers

Product name : 4-(Trifluoromethyl)phenylboronic acid

Product Number : 439320  
Brand : Aldrich  
CAS-No. : 128796-39-4

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

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

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

Company : Sigma-Aldrich Inc.  
3050 SPRUCE ST  
ST. LOUIS MO 63103  
UNITED STATES  
Telephone : +1 314 771-5765  
Fax : +1 800 325-5052

### 1.4 Emergency telephone

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

## SECTION 2: Hazards identification

### 2.1 Classification of the substance or mixture

#### GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)


Acute toxicity, Oral (Category 4), H302

For the full text of the H-Statements mentioned in this Section, see Section 16.

### 2.2 GHS Label elements, including precautionary statements

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Pictogram	
Signal Word	Warning
Hazard Statements H302	Harmful if swallowed.
Precautionary Statements P264 P270 P301 + P312 + P330 P501	Wash skin thoroughly after handling. Do not eat, drink or smoke when using this product. IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth. Dispose of contents/ container to an approved waste disposal plant.

### 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

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## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Synonyms	:	$\alpha,\alpha,\alpha$ -Trifluoro-p-tolylboronic acid 4-(Trifluoromethyl)benzeneboronic acid
Formula	:	$C_7H_6BF_3O_2$
Molecular weight	:	189.93 g/mol
CAS-No.	:	128796-39-4
EC-No.	:	603-301-0

Component	Classification	Concentration
<b>4-(Trifluoromethyl)phenylboronic acid</b>	Acute Tox. 4; H302	<= 100 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

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## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

#### General advice

Show this material safety data sheet to the doctor in attendance.

#### If inhaled

After inhalation: fresh air.

#### In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.

#### In case of eye contact

After eye contact: rinse out with plenty of water. Remove contact lenses.

**If swallowed**

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

**4.2 Most important symptoms and effects, both acute and delayed**

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

**4.3 Indication of any immediate medical attention and special treatment needed**

No data available

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**SECTION 5: Firefighting measures****5.1 Extinguishing media****Suitable extinguishing media**

Water Foam Carbon dioxide (CO<sub>2</sub>) Dry powder

**Unsuitable extinguishing media**

For this substance/mixture no limitations of extinguishing agents are given.

**5.2 Special hazards arising from the substance or mixture**

Carbon oxides

Hydrogen fluoride

Borane/boron oxides

Combustible.

Development of hazardous combustion gases or vapours possible in the event of fire.

**5.3 Advice for firefighters**

In the event of fire, wear self-contained breathing apparatus.

**5.4 Further information**

Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

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**SECTION 6: Accidental release measures****6.1 Personal precautions, protective equipment and emergency procedures**

Advice for non-emergency personnel: Avoid inhalation of dusts. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

For personal protection see section 8.

**6.2 Environmental precautions**

Do not let product enter drains.

**6.3 Methods and materials for containment and cleaning up**

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

**6.4 Reference to other sections**

For disposal see section 13.

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## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

For precautions see section 2.2.

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

#### Storage conditions

Tightly closed. Dry.

#### Storage class

Storage class (TRGS 510): 11: Combustible Solids

### 7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

### 8.2 Exposure controls

#### Appropriate engineering controls

Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

#### Personal protective equipment

##### Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

##### Skin protection

Handle with impervious gloves.

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

##### Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested:KCL 741 Dermatril® L

##### Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested:KCL 741 Dermatril® L

### **Body Protection**

protective clothing

### **Respiratory protection**

Recommended Filter type: Filter type P2

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer.

These measures have to be properly documented.

required when dusts are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

### **Control of environmental exposure**

Do not let product enter drains.

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## **SECTION 9: Physical and chemical properties**

### **9.1 Information on basic physical and chemical properties**

- |   |   |
|---|---|
| a) Appearance                                   | Form: powder<br>Color: white                      |
| b) Odor   | No data available                                 |
| c) Odor Threshold                               | No data available                                 |
| d) pH   | No data available                                 |
| e) Melting point/freezing point                 | Melting point/ range: 245 - 250 °C (473 - 482 °F) |
| f) Initial boiling point and boiling range      | No data available                                 |
| g) Flash point                                  | ( )Not applicable                                 |
| h) Evaporation rate                             | No data available                                 |
| i) Flammability (solid, gas)                    | No data available                                 |
| j) Upper/lower flammability or explosive limits | No data available                                 |
| k) Vapor pressure                               | No data available                                 |
| l) Vapor density                                | No data available                                 |
| m) Density                                      | No data available                                 |
| Relative density                                | No data available                                 |
| n) Water solubility                             | No data available                                 |
| o) Partition coefficient: n-octanol/water       | No data available                                 |

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- |                              |                   |
|------------------------------|-------------------|
| p) Autoignition temperature  | No data available |
| q) Decomposition temperature | No data available |
| r) Viscosity                 | No data available |
| s) Explosive properties      | No data available |
| t) Oxidizing properties      | none              |

## 9.2 Other safety information

No data available

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

### 10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

### 10.3 Possibility of hazardous reactions

No data available

### 10.4 Conditions to avoid

no information available

### 10.5 Incompatible materials

Strong oxidizing agents

### 10.6 Hazardous decomposition products

In the event of fire: see section 5

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## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

Acute toxicity estimate Oral - 500.1 mg/kg

(Expert judgment)

Inhalation: No data available

Dermal: No data available

#### Skin corrosion/irritation

No data available

#### Serious eye damage/eye irritation

No data available

#### Respiratory or skin sensitization

No data available

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**Germ cell mutagenicity**

No data available

**Carcinogenicity**

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

**Reproductive toxicity**

No data available

**Specific target organ toxicity - single exposure**

No data available

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**11.2 Additional Information**

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

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**SECTION 12: Ecological information****12.1 Toxicity**

No data available

**12.2 Persistence and degradability**

No data available

**12.3 Bioaccumulative potential**

No data available

**12.4 Mobility in soil**

No data available

**12.5 Results of PBT and vPvB assessment**

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

**12.6 Endocrine disrupting properties**

No data available

**12.7 Other adverse effects**

No data available

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## **SECTION 13: Disposal considerations**

### **13.1 Waste treatment methods**

#### **Product**

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

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## **SECTION 14: Transport information**

#### **DOT (US)**

Not dangerous goods

#### **IMDG**

Not dangerous goods

#### **IATA**

Not dangerous goods

#### **Further information**

Not classified as dangerous in the meaning of transport regulations.

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## **SECTION 15: Regulatory information**

#### **CERCLA Reportable Quantity**

This material does not contain any components with a CERCLA RQ.

#### **SARA 304 Extremely Hazardous Substances Reportable Quantity**

This material does not contain any components with a section 304 EHS RQ.

#### **SARA 302 Extremely Hazardous Substances Threshold Planning Quantity**

This material does not contain any components with a section 302 EHS TPQ.

**SARA 311/312 Hazards** : Acute Health Hazard

**SARA 313** : This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

#### **US State Regulations**

##### **Massachusetts Right To Know**

No components are subject to the Massachusetts Right to Know Act.



**Massachusetts Right To Know**

No components are subject to the Massachusetts Right to Know Act.

**Pennsylvania Right To Know**

4-(Trifluoromethyl)phenylboronic acid 128796-39-4

**Maine Chemicals of High Concern**

Product does not contain any listed chemicals

**Vermont Chemicals of High Concern**

Product does not contain any listed chemicals

**Washington Chemicals of High Concern**

Product does not contain any listed chemicals

**New Jersey Right To Know**

4-(Trifluoromethyl)phenylboronic acid 128796-39-4

**The ingredients of this product are reported in the following inventories:**

TSCA : Product contains substance(s) not listed on TSCA inventory.

**TSCA list**

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

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**SECTION 16: Other information****Further information**

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See [www.sigma-aldrich.com](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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