

**SECTION 1: Identification of the substance/mixture and of the company/undertaking**

**1.1 Product identifier**  
Trade name **2-Isopropoxy-5-(trifluoromethyl)benzeneboronic acid**  
Stock number: H53121  
CAS Number: 850593-12-3

**1.2 Relevant identified uses of the substance or mixture and uses advised against.**  
Identified use: SU24 Scientific research and development

**1.3 Details of the supplier of the safety data sheet**  
Manufacturer/Supplier: Alfa Aesar GmbH & Co.KG  
A Johnson Matthey Company  
Zeppelinstr. 7b  
76185 Karlsruhe / Germany  
Tel: +49 (0) 721 84007 280  
Fax: +49 (0) 721 84007 300  
Email: tech@alfa.com  
www.alfa.com

**Informing department:** Product safety Tel + +049 (0) 7275 988687-0  
**1.4 Emergency telephone number:** Carechem 24: +44 (0) 1235 239 670 (Multi-language emergency number)  
Poison Information Center Mainz  
www.giftinfo.uni-mainz.de Telephone: +49(0)6131/19240

**SECTION 2: Hazards identification**

**2.1 Classification of the substance or mixture**  
Classification according to Regulation (EC) No 1272/2008



GHS07

Skin Irrit. 2 H315 Causes skin irritation.  
Eye Irrit. 2 H319 Causes serious eye irritation.  
STOT SE 3 H335 May cause respiratory irritation.

**Classification according to Directive 67/548/EEC or Directive 1999/45/EC**

Xi; Irritant

R36/37/38: Irritating to eyes, respiratory system and skin.

**Information concerning particular hazards for human and environment:** Not applicable

**Other hazards that do not result in classification** No information known.

**2.2 Label elements**  
Labelling according to Regulation (EC) No 1272/2008

Hazard pictograms  
Signal word  
Hazard statements

**Precautionary statements**

The substance is classified and labelled according to the CLP regulation.  
GHS07  
Warning  
H315 Causes skin irritation.  
H319 Causes serious eye irritation.  
H335 May cause respiratory irritation.  
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.  
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.  
P302+P352 IF ON SKIN: Wash with plenty of soap and water.  
P321 Specific treatment (see on this label).  
P405 Store locked up.  
P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

**2.3 Other hazards**

**Results of PBT and vPvB assessment**

PBT: Not applicable.  
vPvB: Not applicable.

**SECTION 3: Composition/information on ingredients**

**3.1 Substances**

CAS# Designation: 850593-12-3 2-Isopropoxy-5-(trifluoromethyl)benzeneboronic acid

**SECTION 4: First aid measures**

**4.1 Description of first aid measures**

**After inhalation**

Supply fresh air. If required, provide artificial respiration. Keep patient warm. Consult doctor if symptoms persist.

**After skin contact**

Seek immediate medical advice.  
Instantly wash with water and soap and rinse thoroughly.

**After eye contact**

Seek immediate medical advice.  
Rinse opened eye for several minutes under running water. Then consult doctor.

**After swallowing**

Seek medical treatment.

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

No further relevant information available.

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

No further relevant information available.

**SECTION 5: Firefighting measures**

**5.1 Extinguishing media**

CO<sub>2</sub>, extinguishing powder or water jet. Fight larger fires with water jet or alcohol-resistant foam.

**Suitable extinguishing agents**

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

If this product is involved in a fire, the following can be released:  
Carbon monoxide and carbon dioxide  
Hydrogen fluoride (HF)  
Boron oxide

**5.3 Advice for firefighters**

Wear self-contained breathing apparatus.  
Wear full protective suit.

**Protective equipment:**

**SECTION 6: Accidental release measures**

**6.1 Personal precautions, protective equipment and emergency procedures**

Wear protective equipment. Keep unprotected persons away.  
Ensure adequate ventilation

**6.2 Environmental precautions:**

Do not allow material to be released to the environment without proper governmental permits.  
Do not allow product to reach sewage system or water bodies.  
Do not allow to enter the ground/soil.

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**6.3 Methods and material for containment and cleaning up:**  
**Prevention of secondary hazards:**  
**6.4 Reference to other sections**

Ensure adequate ventilation.  
No special measures required.  
See Section 7 for information on safe handling  
See section 8 for information on personal protection equipment.  
See Section 13 for information on disposal.

**SECTION 7: Handling and storage**

**7.1 Precautions for safe handling**

Keep containers tightly sealed.  
Store in cool, dry place in tightly closed containers.  
Ensure good ventilation/exhaustion at the workplace.

**Information about protection against explosions and fires:**

No information known.

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

**Storage**  
**Requirements to be met by storerooms and containers:**

No special requirements.

**Information about storage in one common storage facility:**

Store away from oxidizing agents.

**Further information about storage conditions:**

Keep container tightly sealed.  
Store in cool, dry conditions in well sealed containers.  
No further relevant information available.

**7.3 Specific end use(s)**

**SECTION 8: Exposure controls/personal protection**

**Additional information about design of technical systems:**

Properly operating chemical fume hood designed for hazardous chemicals and having an average face velocity of at least 100 feet per minute.

**8.1 Control parameters**

**Components with critical values that require monitoring at the workplace:**

The product does not contain any relevant quantities of materials with critical values that have to be monitored at the workplace.

**Additional information:**

No data

**8.2 Exposure controls**

**Personal protective equipment**  
**General protective and hygienic measures**

The usual precautionary measures should be adhered to in handling the chemicals.  
Keep away from foodstuffs, beverages and food.  
Instantly remove any soiled and impregnated garments.  
Wash hands during breaks and at the end of the work.  
Avoid contact with the eyes and skin.  
Maintain an ergonomically appropriate working environment.  
Use breathing protection with high concentrations.  
Check protective gloves prior to each use for their proper condition.  
The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer.

**Breathing equipment:**

**Protection of hands:**

**Material of gloves**

**Penetration time of glove material**

**Eye protection:**

**Body protection:**

Impervious gloves  
Not determined  
Safety glasses  
Face protection  
Protective work clothing.

**SECTION 9: Physical and chemical properties**

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

**General Information**

**Appearance:**

**Form:** Solid.  
**Colour:** White  
**Smell:** Not determined  
**Odour threshold:** Not determined.

**pH-value:** Not applicable.

**Change in condition**

**Melting point/Melting range:** 66-68 °C  
**Boiling point/Boiling range:** Not determined  
**Sublimation temperature / start:** Not determined  
**Inflammability (solid, gaseous)** Not determined.  
**Ignition temperature:** Not determined  
**Decomposition temperature:** Not determined  
**Self-inflammability:** Not determined.

**Critical values for explosion:**

**Lower:** Not determined  
**Upper:** Not determined  
**Steam pressure:** Not applicable.  
**Density** Not determined  
**Relative density** Not determined.  
**Vapour density** Not applicable.  
**Evaporation rate** Not applicable.

**Solubility in / Miscibility with**

**Water:** Not determined  
**Partition coefficient (n-octanol/water):** Not determined.

**Viscosity:**

**dynamic:** Not applicable.  
**kinematic:** Not applicable.

**9.2 Other information** No further relevant information available.

**SECTION 10: Stability and reactivity**

**10.1 Reactivity**

**10.2 Chemical stability**

**Thermal decomposition / conditions to be avoided:**

**10.3 Possibility of hazardous reactions**

**10.5 Incompatible materials:**

**10.6 Hazardous decomposition products:**

No information known.  
Stable under recommended storage conditions.  
No decomposition if used and stored according to specifications.  
No dangerous reactions known  
Oxidizing agents  
Carbon monoxide and carbon dioxide

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 Hydrogen fluoride  
 Boron oxide

**SECTION 11: Toxicological information**
**11.1 Information on toxicological effects**

<b>Acute toxicity:</b>	No effects known.
<b>LD/LC50 values that are relevant for classification:</b>	No data
<b>Skin irritation or corrosion:</b>	Causes skin irritation.
<b>Eye irritation or corrosion:</b>	Causes serious eye irritation.
<b>Sensitization:</b>	No sensitizing effect known.
<b>Germ cell mutagenicity:</b>	No effects known.
<b>Carcinogenicity:</b>	EPA-I: Data are inadequate for an assessment of human carcinogenic potential.
<b>Reproductive toxicity:</b>	No effects known.
<b>Specific target organ system toxicity - repeated exposure:</b>	No effects known.
<b>Specific target organ system toxicity - single exposure:</b>	May cause respiratory irritation.
<b>Aspiration hazard:</b>	No effects known.
<b>Additional toxicological information:</b>	To the best of our knowledge the acute and chronic toxicity of this substance is not fully known.

**SECTION 12: Ecological information**
**12.1 Toxicity**
**Aquatic toxicity:** No further relevant information available.

**12.2 Persistence and degradability** No further relevant information available.

**12.3 Bioaccumulative potential** No further relevant information available.

**12.4 Mobility in soil** No further relevant information available.

**Additional ecological information:**
**General notes:** Do not allow material to be released to the environment without proper governmental permits.  
 Water hazard class 1 (Self-assessment): slightly hazardous for water.  
 Do not allow undiluted product or large quantities of it to reach ground water, water bodies or sewage system.  
 Avoid transfer into the environment.

**12.5 Results of PBT and vPvB assessment**
**PBT:** Not applicable.

**vPvB:** Not applicable.

**12.6 Other adverse effects** No further relevant information available.

**SECTION 13: Disposal considerations**
**13.1 Waste treatment methods**
**Recommendation** Hand over to disposers of hazardous waste.  
 Must be specially treated under adherence to official regulations.  
 Consult state, local or national regulations for proper disposal.

**Uncleaned packagings:**
**Recommendation:** Disposal must be made according to official regulations.

**SECTION 14: Transport information**
**UN-Number**
**ADR, ADN, IMDG, IATA** Not applicable

**14.2 UN proper shipping name**
**ADR, ADN, IMDG, IATA** Not applicable

**14.3 Transport hazard class(es)**
**ADR, ADN, IMDG, IATA** Not applicable

**Class**
**ADR, IMDG, IATA** Not applicable

**Packing group**
**ADR, IMDG, IATA** Not applicable

**14.5 Environmental hazards:** Not applicable.

**14.6 Special precautions for user** Not applicable.

**14.7 Transport in bulk according to Annex II of MARPOL73/78 and the IBC**
**Code** Not applicable.

**UN "Model Regulation":**

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**SECTION 15: Regulatory information**
**15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture**
**Australian Inventory of Chemical**
**Substances** Substance is not listed.

**Standard for the Uniform Scheduling of** Substance is not listed.

**Drugs and Poisons** Substance is not listed.

**National regulations** Substance is not listed.

**Information about limitation of use:** For use only by technically qualified individuals.  
 Employment restrictions concerning young persons must be observed.

**Water hazard class:** Water hazard class 1 (Self-assessment): slightly hazardous for water.

**Other regulations, limitations and prohibitive regulations**
**ELINCS (European List of Notified Chemical** Substance is not listed.

**Substances)** Substance is not listed.

**Substances of very high concern (SVHC)** Substance is not listed.

**according to REACH, Article 57** Substance is not listed.

**REACH - Pre-registered substances** Substance is not listed.

**15.2 Chemical safety assessment:** A Chemical Safety Assessment has not been carried out.

**SECTION 16: Other information**

Employers should use this information only as a supplement to other information gathered by them, and should make independent judgement of suitability of this information to ensure proper use and protect the health and safety of employees. This information is furnished without warranty, and any use of the product not in conformance with this Material Safety Data Sheet, or in combination with any other product or process, is the responsibility of the user.

**Department issuing data specification sheet:** Health, Safety and Environmental Department.

**Abbreviations and acronyms:** RID: Règlement international concernant le transport des marchandises dangereuses par chemin de fer (Regulations Concerning the International Transport of Dangerous Goods by Rail)

ICAO: International Civil Aviation Organization

ADR: Accord européen sur le transport des marchandises dangereuses par Route (European Agreement concerning the International Carriage of Dangerous Goods by Road)

IMDG: International Maritime Code for Dangerous Goods

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DE/E

**Safety data sheet**  
according to 1907/2006/EC, Article 31

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**Trade name 2-Isopropoxy-5-(trifluoromethyl)benzeneboronic acid**

IATA: International Air Transport Association  
GHS: Globally Harmonized System of Classification and Labelling of Chemicals  
CAS: Chemical Abstracts Service (division of the American Chemical Society)  
LC50: Lethal concentration, 50 percent  
LD50: Lethal dose, 50 percent

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