

SAFETY DATA SHEET

Creation Date 04-April-2011 Revision Date 25-August-2023 Revision Number 3

1. Identification

Product Name 1-(tert-Butoxycarbonyl)-5-(trifluoromethoxy)indole-2-boronic acid

Cat No. : MO08435DA; MO08435DE; MO08435ZZ

Synonyms No information available

Recommended Use Laboratory chemicals.

Uses advised against Food, drug, pesticide or biocidal product use.

Details of the supplier of the safety data sheet

Company

Importer/Distributor
Fisher Scientific
One Reagent Lane
112 Colonnade Road,
Ottawa, ON K2E 7L6.
Fisher Scientific
One Reagent Lane
Fair Lawn, NJ 07410

Canada

Tel: 1-800-234-7437

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

2. Hazard(s) identification

Classification

WHMIS 2015 Classification Classified as hazardous under the Hazardous Products Regulations (SOR/2015-17)

Acute oral toxicity
Category 4
Acute dermal toxicity
Category 4
Acute Inhalation Toxicity
Skin Corrosion/Irritation
Category 2
Serious Eye Damage/Eye Irritation
Category 2
Specific target organ toxicity (single exposure)
Category 3

Target Organs - Respiratory system.

Label Elements

Signal Word

Warning

Hazard Statements

Harmful if swallowed, in contact with skin or if inhaled

1-(tert-Butoxycarbonyl)-5-(trifluoromethoxy)indole-2-b oronic acid

Causes skin irritation
Causes serious eye irritation
May cause respiratory irritation



Precautionary Statements

Prevention

Avoid breathing dust/fume/gas/mist/vapors/spray

Wash face, hands and any exposed skin thoroughly after handling

Do not eat, drink or smoke when using this product

Use only outdoors or in a well-ventilated area

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

Response

IF ON SKIN: Wash with plenty of soap and water

IF INHALED: Remove person to fresh air and keep comfortable for breathing

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing Call a POISON CENTER/ doctor if you feel unwell

Rinse mouth

Take off contaminated clothing and wash it before reuse

Storage

Store in a well-ventilated place. Keep container tightly closed

Store locked up

Disposal

Dispose of contents/container to an approved waste disposal plant

3. Composition/Information on Ingredients

| Component | CAS-No | Weight % |
|--|--------------|----------|
| [1-[(2-Methylpropan-2-yl)oxycarbonyl]-5-(trifluorome | 1034566-16-9 | >95 |
| thoxy)indol-2-yl]boronic acid | | |

4. 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.

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

symptoms occur.

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

symptoms occur.

Most important symptoms/effects

Notes to Physician

None reasonably foreseeable.

Treat symptomatically

5. Fire-fighting measures

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

Unsuitable Extinguishing Media No information available

Flash Point No information available Method -No information available

Autoignition Temperature

Explosion Limits

No information available

Upper No data available No data available Lower Sensitivity to Mechanical Impact No information available Sensitivity to Static Discharge No information available

Specific Hazards Arising from the Chemical

Keep product and empty container away from heat and sources of ignition.

Hazardous Combustion Products

Carbon monoxide (CO). Carbon dioxide (CO₂). Nitrogen oxides (NOx). Oxides of boron. Hydrogen fluoride. Fluorine.

Protective Equipment and Precautions for Firefighters

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

NFPA

| Health | Flammability | Instability | Physical hazards |
|--------|--------------|-------------|------------------|
| 2 | 1 | 0 | N/A |

Accidental release measures

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

formation.

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

Information.

Methods for Containment and Clean Sweep up and shovel into suitable containers for disposal. Keep in suitable, closed Up

containers for disposal.

| | 7. Handling and storage |
|----------|---|
| Handling | Wear personal protective equipment/face protection. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation. Ensure adequate ventilation. Avoid dust formation. |
| Storage. | Keep containers tightly closed in a dry, cool and well-ventilated place. Incompatible Materials. Strong oxidizing agents. Strong reducing agents. Strong acids. Strong bases. |

8. Exposure controls / personal protection

This product does not contain any hazardous materials with occupational exposure **Exposure Guidelines**

limitsestablished by the region specific regulatory bodies.

Engineering Measures Use only under a chemical fume hood. 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

Hand Protection Wear appropriate protective gloves and clothing to prevent skin exposure.

| Glove material | Breakthrough time | Glove thickness | Glove comments |
|----------------|-------------------|-----------------|------------------------|
| Natural rubber | See manufacturers | - | Splash protection only |
| Butyl rubber | recommendations | | |
| Nitrile rubber | | | |
| Neoprene | | | |
| PVC | | | |

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. Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced. To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly **Recommended Filter type:** Particulates filter conforming to EN 143

When RPE is used a face piece Fit Test should be conducted

Environmental exposure controls

No information available.

Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Wash hands before breaks and after work.

9. Physical and chemical properties

Physical State Solid Appearance White

OdorNo information availableOdor ThresholdNo information availablepHNo information available

Melting Point/Range 89 - 99 °C / 192.2 - 210.2 °F

Boiling Point/Range
No information available
No information available
No information available

Evaporation Rate Not applicable

Flammability (solid,gas) No information available

Flammability or explosive limits

UpperNo data availableLowerNo data availableVapor PressureNo information availableVapor DensityNot applicable

Vapor DensityNot applicableSpecific GravityNo information availableSolubilityNo information availablePartition coefficient; n-octanol/waterNo data available

Autoignition Temperature

No information available

Decomposition Temperature

No information available

Viscosity Not applicable

1-(tert-Butoxycarbonyl)-5-(trifluoromethoxy)indole-2-b oronic acid

Molecular Formula C14H15BF3NO5

Molecular Weight 345.08

10. Stability and reactivity

Reactive Hazard None known, based on information available

Stability Stable under normal conditions.

Conditions to Avoid Incompatible products. Excess heat. Avoid dust formation.

Incompatible Materials Strong oxidizing agents, Strong reducing agents, Strong acids, Strong bases

Hazardous Decomposition Products Carbon monoxide (CO), Carbon dioxide (CO₂), Nitrogen oxides (NOx), Oxides of boron,

Hydrogen fluoride, Fluorine

Hazardous Polymerization Hazardous polymerization does not occur.

Hazardous ReactionsNone under normal processing.

11. Toxicological information

Acute Toxicity

Product Information Component Information

Toxicologically Synergistic

Products

No information available

Delayed and immediate effects as well as chronic effects from short and long-term exposure

Irritation No information available

Sensitization No information available

Carcinogenicity The table below indicates whether each agency has listed any ingredient as a carcinogen.

| Component | CAS-No | IARC | NTP | ACGIH | OSHA | Mexico |
|---------------------------|--------------|------------|------------|------------|------------|------------|
| [1-[(2-Methylpropan-2- | 1034566-16-9 | Not listed |
| yl)oxycarbonyl]-5-(triflu | | | | | | |
| oromethoxy)indol-2-yl] | | | | | | |
| boronic acid | | | | | | |

Mutagenic Effects No information available

Reproductive Effects No information available.

Developmental Effects No information available.

Teratogenicity No information available.

STOT - single exposure Respiratory system STOT - repeated exposure None known

Aspiration hazard No information available

Symptoms / effects,both acute and No information available

delayed

Endocrine Disruptor Information No information available

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

12. Ecological information

Ecotoxicity

Do not empty into drains.

Persistence and DegradabilitySoluble in water Persistence is unlikely based on information available.

Bioaccumulation/ Accumulation No information available.

Mobility Will likely be mobile in the environment due to its water solubility.

13. Disposal considerations

Waste Disposal Methods Chemical waste generators must determine whether a discarded chemical is classified as a

hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

14. Transport information

DOT

UN-No UN2811

Proper Shipping Name TOXIC SOLIDS, ORGANIC, N.O.S.

Hazard Class 6.1 Packing Group III

<u>TDG</u>

UN-No UN2811

Proper Shipping Name Toxic solid, organic, n.o.s.

Hazard Class 6.1 Packing Group

IATA

UN-No UN2811

Proper Shipping Name Toxic solid, organic, n.o.s.

Hazard Class 6.1 Packing Group III

IMDG/IMO

UN-No UN2811

Proper Shipping Name Toxic solid, organic, n.o.s.

Hazard Class 6.1
Packing Group

15. Regulatory information

International Inventories

| Component | CAS-No | DSL | NDSL | TSCA | TSCA Inventory notification - Active-Inactive | EINECS | ELINCS | NLP |
|---------------------------------------|--------------|-----|------|------|---|--------|--------|-----|
| [1-[(2-Methylpropan-2-yl)oxycarbo | 1034566-16-9 | - | - | - | - | - | - | - |
| nyl]-5-(trifluoromethoxy)indol-2-yl]b | | | | | | | | |
| oronic acid | | | | | | | | |

| Component | CAS-No | IECSC | KECL | ENCS | ISHL | TCSI | AICS | NZIoC | PICCS |
|---------------------------------------|--------------|-------|------|------|------|------|------|-------|-------|
| [1-[(2-Methylpropan-2-yl)oxycarbo | 1034566-16-9 | - | - | - | - | - | - | - | - |
| nyl]-5-(trifluoromethoxy)indol-2-yl]b | | | | | | | | | |
| oronic acid | | | | | | | | | |

Legend:

X - Listed '-' - Not Listed

KECL - NIER number or KE number (http://ncis.nier.go.kr/en/main.do)

DSL/NDSL - Canadian Domestic Substances List/Non-Domestic Substances List

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

1-(tert-Butoxycarbonyl)-5-(trifluoromethoxy)indole-2-b oronic acid

EINECS/ELINCS - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

IECSC - Chinese Inventory of Existing Chemical Substances **KECL** - Korean Existing and Evaluated Chemical Substances

ENCS - Japanese Existing and New Chemical Substances

AICS - Australian Inventory of Chemical Substances

PICCS - Philippines Inventory of Chemicals and Chemical Substances

Canada

SDS in compliance with provisions of information as set out in Canadian Standard - Part 4, Schedule 1 and 2 of the Hazardous Products Regulations (HPR) and meets the requirements of the HPR (Paragraph 13(1)(a) of the Hazardous Products Act (HPA)).

Other International Regulations

Authorisation/Restrictions according to EU REACH

Not applicable

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

| Component | CAS-No | OECD HPV | Persistent Organic Pollutant | Ozone Depletion Potential | Restriction of Hazardous Substances (RoHS) |
|---|--------|----------------|---------------------------------|------------------------------|--|
| [1-[(2-Methylpropan-2-yl)oxyc arbonyl]-5-(trifluoromethoxy)in dol-2-yl]boronic acid | | Not applicable | Not applicable | Not applicable | Not applicable |

| 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 | Rotterdam Convention (PIC) | Basel Convention (Hazardous Waste) |
|---|--------|---|--|-------------------------------|---------------------------------------|
| [1-[(2-Methylpropan-2-yl)oxyc arbonyl]-5-(trifluoromethoxy)in dol-2-yl]boronic acid | | Not applicable | Not applicable | Not applicable | Not applicable |

16. Other information

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Revision Summary

This document has been updated to comply with the requirements of WHMIS 2015 to align

with the Globally Harmonised System (GHS) for the Classification and Labelling of

Chemicals.

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 SDS