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

1.1 Product identifiers

Product name: Boron trifluoride diethyl etherate
Product Number: 216607
Brand: Aldrich
CAS-No.: 109-63-7

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

Identified uses: Laboratory chemicals, Synthesis of substances
Uses advised against:

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)

Flammable liquids (Category 3), H226
Acute toxicity, Oral (Category 4), H302
Acute toxicity, Inhalation (Category 4), H332
Skin corrosion (Category 1B), H314
Serious eye damage (Category 1), H318
Specific target organ toxicity - repeated exposure, Inhalation (Category 1), Kidney, H372

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

2.2 GHS Label elements, including precautionary statements
2.3 Hazards not otherwise classified (HNOC) or not covered by GHS
Strong hydrogen fluoride releaser
Reacts violently with water.

SECTION 3: Composition/information on ingredients

3.1 Substances
Synonyms: Trifluoro[1,1'-oxybis [ethane]]-(T-4)-boron
Boron trifluoride ethyl etherate

Formula: BF₃ · C₄H₁₀O
Molecular weight: 141.93 g/mol
CAS-No.: 109-63-7
EC-No.: 203-689-8

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>boron trifluoride-diethyl ether complex (1:1)</td>
<td>Flam. Liq. 3; Acute Tox. 4; Skin Corr. 1B; Eye Dam. 1; STOT RE 1; H226, H302, H332, H314, H318, H372</td>
<td>&lt;= 100 %</td>
</tr>
</tbody>
</table>

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

SECTION 4: First aid measures

4.1 Description of first-aid measures

**General advice**

Hydrofluoric (HF) acid burns require immediate and specialized first aid and medical treatment. Symptoms may be delayed up to 24 hours depending on the concentration of HF. After decontamination with water, further damage can occur due to penetration/absorption of the fluoride ion. Treatment should be directed toward binding the fluoride ion as well as the effects of exposure. Skin exposures can be treated with a 2.5% calcium gluconate gel repeated until burning ceases. More serious skin exposures may require subcutaneous calcium gluconate except for digital areas unless the physician is experienced in this technique, due to the potential for tissue injury from increased pressure. Absorption can readily occur through the subungual areas and should be considered when undergoing decontamination. Prevention of absorption of the fluoride ion in cases of ingestion can be obtained by giving milk, chewable calcium carbonate tablets or Milk of Magnesia to conscious victims. Conditions such as hypocalcemia, hypomagnesemia and cardiac arrhythmias should be monitored for, since they can occur after exposure. First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

**If inhaled**

After inhalation: fresh air. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

**In case of skin contact**

First treatment with calcium gluconate paste. In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/shower. Call a physician immediately.

**In case of eye contact**

After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist. Remove contact lenses.
If swallowed
After swallowing: make victim drink water (two glasses at most), avoid vomiting (risk of perforation). Call a physician immediately. Do not attempt to neutralise.

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

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media
Carbon dioxide (CO2) Dry powder Cover with dry sand or cement.

Unsuitable extinguishing media
Foam Water

5.2 Special hazards arising from the substance or mixture
Carbon oxides
Hydrogen fluoride
Borane/boron oxides
Combustible.
Vapors are heavier than air and may spread along floors.
Forms explosive mixtures with air at elevated temperatures.
Development of hazardous combustion gases or vapours possible in the event of fire.

5.3 Advice for firefighters
Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 Further information
Water hydrolyzes material liberating acidic gas which in contact with metal surfaces can generate flammable and/or explosive hydrogen gas. Remove container from danger zone and cool with water. Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures
Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. 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. Risk of explosion.
6.3 Methods and materials for containment and cleaning up
Contain spillage, soak up with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and transfer to a container for disposal according to local / national regulations (see section 13). Large spills should be collected mechanically (remove by pumping) for disposal. Do not flush with water. Ventilate the area. Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections
For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling
Advice on safe handling
Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Advice on protection against fire and explosion
Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures
Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.
For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities
Storage conditions
Store under nitrogen. Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition. Keep locked up or in an area accessible only to qualified or authorized persons. Keep away from water.

Storage stability
Recommended storage temperature
2 - 8 °C
Store under inert gas. Do not store in glass

Storage class
Storage class (TRGS 510): 3: Flammable liquids

7.3 Specific end use(s)
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

8.1 Control parameters
Ingredients with workplace control parameters
8.2 Exposure controls

Appropriate engineering controls
Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face 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). Tightly fitting safety goggles.

Skin protection
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 EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Full contact
Material: Nitrile rubber
Minimum layer thickness: 0.4 mm
Break through time: 480 min
Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

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 EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Splash contact
Material: Viton®
Minimum layer thickness: 0.7 mm
Break through time: 120 min
Material tested: Vitoject® (KCL 890 / Aldrich Z677698, Size M)

Body Protection
Flame retardant antistatic protective clothing.

Respiratory protection
Recommended Filter type: Filter type B
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 vapours/aerosols 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.

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Value</th>
<th>Control parameters</th>
<th>Basis</th>
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<tbody>
<tr>
<td>boron trifluoride-diethyl ether complex (1:1)</td>
<td>109-63-7</td>
<td>TWA</td>
<td>0.1 ppm</td>
<td>USA. ACGIH Threshold Limit Values (TLV)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>C</td>
<td>0.7 ppm</td>
<td>USA. ACGIH Threshold Limit Values (TLV)</td>
</tr>
</tbody>
</table>
Control of environmental exposure
Do not let product enter drains. Risk of explosion.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Details</th>
</tr>
</thead>
</table>
| a) Appearance | Form: liquid  
Color: slightly opalescent, yellow |
| b) Odor | No data available |
| c) Odor Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | Melting point/range: -58 °C (-72 °F) - lit. |
| f) Initial boiling point and boiling range | 126 - 129 °C 259 - 264 °F - lit. |
| g) Flash point | 58.5 °C (137.3 °F) - closed cup - Regulation (EC) No. 440/2008, Annex, A.9 |
| h) Evaporation rate | No data available |
| i) Flammability (solid, gas) | No data available |
| j) Upper/lower flammability or explosive limits | Upper explosion limit: 36 % (V)  
Lower explosion limit: 1.9 % (V) |
| k) Vapor pressure | 2.7 hPa at 20 °C (68 °F) |
| l) Vapor density | 4.90 - (Air = 1.0) |
| m) Density | 1.15 g/cm3 - lit.  
Relative density 1.12525 °C |
| n) Water solubility | No data available |
| o) Partition coefficient: n-octanol/water | No data available |
| p) Autoignition temperature | No data available |
| q) Decomposition temperature | No data available |
| r) Viscosity | No data available |
| s) Explosive properties | None |
| t) Oxidizing properties | None |

9.2 Other safety information

<table>
<thead>
<tr>
<th>Property</th>
<th>Details</th>
</tr>
</thead>
<tbody>
<tr>
<td>Relative vapor density</td>
<td>4.90 - (Air = 1.0)</td>
</tr>
</tbody>
</table>
SECTION 10: Stability and reactivity

10.1 Reactivity
Vapor/air-mixtures are explosive at intense warming.

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

10.3 Possibility of hazardous reactions
Risk of explosion with:
lithium aluminium hydride
Risk of ignition or formation of inflammable gases or vapours with:
Alkali metals
Water
Acids
Violent reactions possible with:
Oxidizing agents
Alcohols
alkalines

10.4 Conditions to avoid
Water hydrolyzes material liberating acidic gas which in contact with metal surfaces can generate flammable and/or explosive hydrogen gas. Do not allow water to enter container because of violent reaction.
Reacts dangerously with glass.
Heating.

10.5 Incompatible materials
glass

10.6 Hazardous decomposition products
In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity
LD50 Oral - Rat - male and female - 326 mg/kg
Remarks: (External MSDS)
The value is given in analogy to the following substances: Boron trifluoride dihydrate
LC50 Inhalation - Rat - male and female - 4 h - 1.21 mg/l - aerosol

(OECD Test Guideline 403)
Remarks: The value is given in analogy to the following substances: Boron trifluoride dihydrate

Dermal: No data available
Skin corrosion/irritation
Skin - Rabbit
Result: Causes burns.
Remarks: (ECHA)

Serious eye damage/eye irritation
Eyes - Rabbit
Result: Corrosive
Remarks: (External MSDS)

Respiratory or skin sensitization
No data available

Germ cell mutagenicity
Test Type: Ames test
Test system: Salmonella typhimurium
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 471
Result: negative
Test Type: In vitro mammalian cell gene mutation test
Test system: mouse lymphoma cells
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 476
Result: negative
Test Type: Chromosome aberration test in vitro
Test system: lymphocyte
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 473
Result: negative

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
Inhalation - The substance or mixture is classified as specific target organ toxicant, repeated exposure, category 1.
- Kidney

Aspiration hazard
No data available

11.2 Additional Information
Fluoride ion can reduce serum calcium levels possibly causing fatal hypocalcemia.
Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea, Vomiting
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Liver - Irregularities - Based on Human Evidence

Liver - Irregularities - Based on Human Evidence

---

SECTION 12: Ecological information

12.1 Toxicity
No data available

12.2 Persistence and degradability
Biodegradability
- aerobic - Exposure time 28 d
  Result: 2.5 % - Not readily biodegradable.
  (OECD Test Guideline 301C)

12.3 Bioaccumulative potential
Bioaccumulation
- Cyprinus carpio (Carp)(boron trifluoride-diethyl ether complex (1:1))
  Bioconcentration factor (BCF): > 0.9 - < 1.4
  (OECD Test Guideline 305C)

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

---

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.


**SECTION 14: Transport information**

**DOT (US)**
- UN number: 2604  Class: 8 (3)  Packing group: I
- Proper shipping name: Boron trifluoride diethyl etherate
- Reportable Quantity (RQ):
  - Poison Inhalation Hazard: No

**IMDG**
- UN number: 2604  Class: 8 (3)  Packing group: I
- EMS-No: F-E, S-C
- Proper shipping name: BORON TRIFLUORIDE DIETHYL ETHERATE

**IATA**
- UN number: 2604  Class: 8 (3)  Packing group: I
- Proper shipping name: Boron trifluoride diethyl etherate

**SECTION 15: Regulatory information**

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

**SARA 313 Components**
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.

**SARA 311/312 Hazards**
Fire Hazard, Acute Health Hazard, Chronic Health Hazard

**Massachusetts Right To Know Components**

<table>
<thead>
<tr>
<th>Compound</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>boron trifluoride-diethyl ether complex (1:1)</td>
<td>109-63-7</td>
<td>1993-04-24</td>
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</table>

**Pennsylvania Right To Know Components**

<table>
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<th>Compound</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
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<td>boron trifluoride-diethyl ether complex (1:1)</td>
<td>109-63-7</td>
<td>1993-04-24</td>
</tr>
</tbody>
</table>
SECTION 16: Other information

Further information
The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. 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 and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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Version: 6.9  Revision Date: 08/02/2023  Print Date: 08/12/2023