

SAFETY DATA SHEET

Version 6.11
Revision Date 04/28/2025
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SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : 1-Chloromethyl-4-fluoro-1,4-diazoniabicyclo[2.2.2]octane bis(tetrafluoroborate)

Product Number : 439479
Brand : Aldrich
Index-No. : 005-015-00-6
CAS-No. : 140681-55-6

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

GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

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The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada

**MILLIPORE
SIGMA**

Acute toxicity (Oral) : Category 4

Serious eye damage : Category 1

Skin sensitization : Category 1

Short-term (acute) aquatic hazard : Category 3

Long-term (chronic) aquatic hazard : Category 3

Other hazards

None known.

GHS label elements

Hazard pictograms :



Signal Word : Danger

Hazard Statements : H302 Harmful if swallowed.
H317 May cause an allergic skin reaction.
H318 Causes serious eye damage.
H412 Harmful to aquatic life with long lasting effects.

Precautionary Statements :

Prevention:

P261 Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.

P264 Wash skin thoroughly after handling.

P270 Do not eat, drink or smoke when using this product.

P272 Contaminated work clothing must not be allowed out of the workplace.

P273 Avoid release to the environment.

P280 Wear protective gloves/ eye protection/ face protection.

Response:

P301 + P312 + P330 IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.

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

P305 + P351 + P338 + P310 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor.

P333 + P313 If skin irritation or rash occurs: Get medical advice/ attention.

P363 Wash contaminated clothing before reuse.

Disposal:

P501 Dispose of contents/ container to an approved waste disposal plant.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

Components

| Chemical name | CAS No./Unique ID | Concentration (% w/w) | Trade secret |
|--|-------------------|-----------------------|--------------|
| 1-(Chloromethyl)-4-fluoro-1,4-diazoniabicyclo[2.2.2]octane ditetrafluoroborate | 140681-55-6* | >= 90 - <= 100 | - |

* Indicates that the identifier is a CAS No.

Actual concentration is withheld as a trade secret

SECTION 4. 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. Consult a physician.
Move out of dangerous area.
Show this material safety data sheet to the doctor in attendance.
Hydrofluoric (HF) acid burns require immediate and

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

| | |
|---|---|
| If inhaled | : After inhalation: fresh air. |
| 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. Consult a physician. |
| 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: immediately make victim drink water (two glasses at most). Consult a physician. |
| 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 |
| Protection of first-aiders | : For personal protection see section 8. |
| Notes to physician | : No data available |

SECTION 5. FIRE-FIGHTING MEASURES

| | |
|------------------------------|-----------------|
| Suitable extinguishing media | : Water Foam |
|------------------------------|-----------------|

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Carbon dioxide (CO₂)
Dry powder

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

Specific hazards during fire fighting : Combustible.

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

Hazardous combustion products : Carbon oxides

Nitrogen oxides (NO_x)

Hydrogen chloride gas

Hydrogen fluoride

Borane/boron oxides

Specific extinguishing methods : No data available

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.

Special protective equipment for fire-fighters : Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

SECTION 6. ACCIDENTAL RELEASE MEASURES

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

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procedures, consult an expert.
Advice for emergency responders:
For personal protection see section 8.

- Environmental precautions : Do not let product enter drains.
- 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.

SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

- Further information on storage conditions : Tightly closed.
Dry.
- Storage class : 11, Combustible Solids
- Recommended storage temperature : 36 - 46 °F / 2 - 8 °C
- Further information on storage stability : Handle and store under inert gas.

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

Engineering measures : No data available

Personal protective equipment

Respiratory protection : 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.

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

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the instructions of the producer. These measures have to be properly documented.

Hand protection

Material : Nitrile rubber
Break through time : 480 min
Glove thickness : 0.11 mm
Protective index : Full contact
Manufacturer : KCL 741 Dermatril® L

Material : Nitrile rubber
Break through time : 480 min
Glove thickness : 0.11 mm
Protective index : Splash contact
Manufacturer : KCL 741 Dermatril® L

Remarks : 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).

Eye 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 and body protection : protective clothing

Hygiene measures : Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance : powder

Color : white

Odor : irritating

Odor Threshold : No data available

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| | |
|---|--|
| pH | : No data available |
| Melting point/ range | : 500 °F / 260 °C Method: lit. |
| Boiling point/boiling range | : No data available |
| Flash point | : No data available |
| Evaporation rate | : No data available |
| Flammability (solid, gas) | : No data available |
| Flammability (liquids) | : No data available |
| Burning rate | : No data available |
| Self-ignition | : > 752 °F / > 400 °C Method: Regulation (EC) No. 440/2008, Annex, A.16 GLP: yes |
| Upper explosion limit / Upper flammability limit | : No data available |
| Lower explosion limit / Lower flammability limit | : No data available |
| Vapor pressure | : < 0.1 hPa (77 °F / 25 °C) Method: Regulation (EC) No. 440/2008, Annex, A.4 GLP: yes |
| Relative vapor density | : No data available |
| Relative density | : 1.71 (68 °F / 20 °C) Method: Regulation (EC) No. 440/2008, Annex, A.3 GLP: yes |
| Density | : No data available |
| Solubility(ies) Water solubility | : 176 g/l soluble (68 °F / 20 °C) Method: Regulation (EC) No. 440/2008, Annex, A.6 GLP: yes |
| Partition coefficient: n- octanol/water | : log Pow: -3.39 (68 °F / 20 °C) Method: Regulation (EC) No. 440/2008, Annex, A.8 GLP: yes Bioaccumulation is not expected. |
| Autoignition temperature | : > 752 °F / > 400 °C Method: Tested according to Directive 92/69/EEC. GLP: yes |

| | |
|---|--|
| Decomposition temperature | : No data available |
| Viscosity, dynamic | : No data available |
| Viscosity, kinematic | : No data available |
| Flow time | : No data available |
| Explosive properties | : No data available |
| Oxidizing properties | : none |
| Surface tension | : 73.1 mN/m, 1 g/l, 66 °F / 19 °C, Surface tension, GLP: yes |
| Molecular weight | : 354.26 g/mol |
| Particle characteristics Particle size | : No data available |

SECTION 10. STABILITY AND REACTIVITY

| | |
|------------------------------------|---|
| 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. |
| Chemical stability | : The product is chemically stable under standard ambient conditions (room temperature) . |
| Possibility of hazardous reactions | : No data available |
| Conditions to avoid | : Avoid moisture. no information available |
| Incompatible materials | : Strong oxidizing agents |
| 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 - 500 mg/kg

Remarks: (External MSDS)

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Inhalation: Irritating to respiratory system.
LD50 Dermal - Rat - > 2,000 mg/kg
(Tested according to Directive 92/69/EEC.)

Skin corrosion/irritation

Skin - Rabbit

Result: No eye irritation - 4 h

Remarks: (ECHA)

Serious eye damage/eye irritation

Eyes - Chicken eye

Result: Causes serious eye damage.

Remarks: (ECHA)

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: positive

(Tested according to Directive 92/69/EEC.)

Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

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: Chromosome aberration test in vitro

Test system: Human lymphocytes

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

No data available

Aspiration hazard

No data available

11.2 Additional Information

Repeated dose toxicity - Rat - Oral - 28 Days - NOAEL (No observed adverse effect level) - 15 mg/kg

Remarks: (ECHA)

Fluoride ion can reduce serum calcium levels possibly causing fatal hypocalcemia. Toxicity reported for borates in humans: ingestion or absorption may cause nausea, vomiting, diarrhea, abdominal cramps, and erythematous lesions on the skin and mucous membranes. Other symptoms include: circulatory collapse, tachycardia, cyanosis, delirium, convulsions, and coma. Death has been reported to occur in infants from less than 5 grams and in adults from 5 to 20 grams., Stomach/intestinal disorders, Kidney injury may occur., Drowsiness, fatigue, Dizziness, Ataxia., Hyperactivity., Salivation
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity

Components:

1-(Chloromethyl)-4-fluoro-1,4-diazoniabicyclo[2.2.2]octane ditetrafluoroborate:

Toxicity to fish : LC50 (Oncorhynchus mykiss (rainbow trout)): 100 mg/l
End point: mortality
Exposure time: 96 h
Test Type: static test
Method: Regulation (EC) No. 440/2008, Annex, C.1
GLP: yes

Toxicity to daphnia and other aquatic invertebrates : EC50 (Daphnia magna (Water flea)): 25 mg/l
Exposure time: 48 h
Method: Regulation (EC) No. 440/2008, Annex, C.2
GLP: yes

Toxicity to algae/aquatic plants : ErC50 (Pseudokirchneriella subcapitata): 90 mg/l
Exposure time: 72 h
Method: Regulation (EC) No. 440/2008, Annex, C.3
GLP: yes

Persistence and degradability

Components:

1-(Chloromethyl)-4-fluoro-1,4-diazoniabicyclo[2.2.2]octane ditetrafluoroborate:

Biodegradability : Result: Not readily biodegradable.

Biodegradation: 41 %
Exposure time: 28 d
Method: Directive 67/548/EEC Annex V, C.4.E.
GLP: yes

Bioaccumulative potential

Components:

1-(Chloromethyl)-4-fluoro-1,4-diazoniabicyclo[2.2.2]octane ditetrafluoroborate:

Partition coefficient: n-octanol/water : log Pow: -3.39 (68 °F / 20 °C)
pH: 3.5
Method: Regulation (EC) No. 440/2008, Annex, A.8
GLP: yes
Remarks: Bioaccumulation is not expected.

Mobility in soil

No data available

Other adverse effects

No data available

SECTION 13. DISPOSAL CONSIDERATIONS

Disposal methods

Waste from residues : 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

International Regulations

IATA-DGR

Not regulated as a dangerous good

IMDG-Code

Not regulated as a dangerous good

Transport in bulk according to IMO instruments

Not applicable for product as supplied.

National regulation

49 CFR Road

Not regulated as a dangerous good

Poison Inhalation Hazard : No

Special precautions for user

Remarks : Not classified as dangerous in the meaning of transport regulations.

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 : Reactivity Hazard
Acute Health Hazard
Chronic 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

1-(Chloromethyl)-4-fluoro-1,4-diazoniabicyclo[2.2.2]octane ditetrafluoroborate 140681-55-6

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

1-(Chloromethyl)-4-fluoro-1,4-diazoniabicyclo[2.2.2]octane ditetrafluoroborate 140681-55-6

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

TSCA : All substances listed as active on the 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.

SECTION 16. OTHER INFORMATION

Full text of other abbreviations

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonized System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organization for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

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 and/or the reverse side of invoice or packing slip for

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