

SAFETY DATA SHEET

Version 8.2
Revision Date 2025.07.16
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1. PRODUCT AND COMPANY 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

1.2 Other means of identification

N-Chloromethyl-N'-fluorotriethylenediammonium bis(tetrafluoroborate)
F-TEDA

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

Identified uses : For R&D use only. Not for pharmaceutical, household or other uses.

1.4 Details of the supplier of the safety data sheet

Company :

MERCK LTD.
20F., No. 121, Jingmao 2nd Road, Nangang District, Taipei City
115, Taiwan

Merck KGaA
64271 Darmstadt
Germany
Phone: +49 6151 72-0

1.5 Emergency telephone number

Emergency Phone : +(44)-870-8200418 (CHEMTREC (GB))
Number : +(353)-19014670 (CHEMTREC Ireland)
001-803-017-9114 (CHEMTREC India)

2. HAZARDS IDENTIFICATION

GHS Classification

Acute toxicity (Oral) : Category 4

Serious eye damage/eye irritation : Category 1

Skin sensitisation : Category 1

Short-term (acute) aquatic hazard : Category 3

Long-term (chronic) aquatic hazard : Category 3

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/ vapours/ spray.
P264 Wash skin thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P272 Contaminated work clothing should 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 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 medi-

cal advice/ attention.
P362 + P364 Take off contaminated clothing and wash it before reuse.

Disposal:

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

Other hazards which do not result in classification

None known.

3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

Components

Hazardous ingredients	CAS-No.	Concentration (% w/w)
1-(Chloromethyl)-4-fluoro-1,4-diazoniabicyclo[2.2.2]octane ditetrafluoroborate	140681-55-6	>= 90 -<= 100

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

First aid measures for different exposure routes

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

5. FIREFIGHTING MEASURES

Suitable extinguishing media	: Water Foam
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	Carbon dioxide (CO ₂) 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	: Suppress (knock down) gases/vapours/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.

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

7. HANDLING AND STORAGE

Handling

For precautions see section 2.2.

Storage

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

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

Biological occupational exposure limits

Contains no substances with biological exposure indices.

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 test-

ing of respiratory protective devices are carried out according to 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 : 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.

9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance : powder

Color : white

Odor : irritating

Odor Threshold : No data available

pH : No data available

Melting point/ range	: 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	: > 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 (25 °C) Method: Regulation (EC) No. 440/2008, Annex, A.4 GLP: yes
Relative vapour density	: No data available
Relative density	: 1.71 (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 (20 °C) Method: Regulation (EC) No. 440/2008, Annex, A.6 GLP: yes
Partition coefficient: n- octanol/water	: log Pow: -3.39 (20 °C) Method: Regulation (EC) No. 440/2008, Annex, A.8 GLP: yes Bioaccumulation is not expected.
Autoignition temperature	: > 400 °C Method: Tested according to Directive 92/69/EEC. GLP: yes
Decomposition tempera-	: No data available

ture

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, 19 °C, Surface tension, GLP: yes
Molecular weight	: 354.26 g/mol
Particle characteristics	
Particle size	: No data available

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

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - 500 mg/kg

Remarks: (External MSDS)

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

Maximisation 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

No data available

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 - 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, tachycar-

dia, 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.

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 (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

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.

The chemical must be disposed or recycled in accordance with Waste Disposal Act. See www.epa.gov.tw for the information of chemical waste disposal companies and their contacts.

14. TRANSPORT INFORMATION

International Regulations

IATA-DGR

UN/ID No. : Not applicable
Proper shipping name : Not applicable
Class : Not applicable
Subsidiary risk : Not applicable
Packing group : Not applicable
Labels : Not applicable
Packing instruction (cargo aircraft) : Not applicable
Packing instruction (passenger aircraft) : Not applicable

IMDG-Code

UN number : Not applicable
Proper shipping name : Not applicable
Class : Not applicable

Subsidiary risk	: Not applicable
Packing group	: Not applicable
Labels	: Not applicable
EmS Code	: Not applicable
Marine pollutant	: no

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable for product as supplied.

Special precautions for user

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

National regulatory information

Occupational Safety and Health Act; Regulations on Occupational Safety and Health Facilities	: applicable
Waste Disposal Act; Standards for the Storage, Cleanup, Handling and Disposal of Industrial Waste	: applicable
Regulations on Labelling and Hazard Communication of Hazardous Chemicals; Exposure Assessment and Control Banding of Hazardous Chemicals	: applicable
Rules on Road Traffic Safety	: Not applicable
Standards of Permissible Exposure Limits in Workplace	: Contains no substances with occupational exposure limit values.
Rules on the Prevention of Poisoning from Organic Solvents.	: Not applicable
Standard for the Control of Designated Hazardous and Dangerous Chemicals	: Not applicable
Standards for Establishing Places for Manufacturing, Storing, Processing Public Hazardous Substances and Flammable Pressurized Gases, and Regulations on Safety Control of such Places	: Not applicable
Toxic and Concerned Chemical Substances Control Act	
Toxic chemical substances	: Not applicable
Concerned chemical substances	: Not applicable
Regulations for Governing Designating and Handling of Priority Management Chemicals	: Not applicable

16. OTHER INFORMATION

Further information

Literature references	: About detail information, please refer to each section The information contained herein is based on the pre-
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sent state of our knowledge. It characterises the product with regard to the appropriate safety precautions. It does not represent a guarantee of any properties of the product.

Organization that prepared the SDS : Name:Merck KGaA LS-QH
Address/Telephone number:64271 Darmstadt Germany/+49 6151 72-0

Date that the SDS was prepared : 2025.07.16

Other 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 and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.
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Date format : yyyy/mm/dd

Full text of other abbreviations

AIIC - Australian Inventory of Industrial Chemicals; ANTT - National Agency for Transport by Land of Brazil; ASTM - American Society for the Testing of Materials; bw - Body weight; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; 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 Harmonised System; GLP - Good Laboratory Practice; 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 Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; 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 Pol-

lution from Ships; MERCOSUR - The Agreement for the Facilitation of the Transport of Dangerous Goods; n.o.s. - Not Otherwise Specified; Nch - Chilean Norm; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NOM - Official Mexican Norm; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation 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; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; SADT - Self-Accelerating Decomposition Temperature; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TDG - Transportation of Dangerous Goods; 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; WHMIS - Workplace Hazardous Materials Information System

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