

1. PRODUCT AND COMPANY IDENTIFICATION**1.1 Product identifiers**

Product name : Selectfluor® fluorinating reagent

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

1.3 Details of the supplier of the safety data sheetCompany : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USATelephone : +1 800-325-5832
Fax : +1 800-325-5052**1.4 Emergency telephone number**

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

2. HAZARDS IDENTIFICATION**2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Self-heating substances and mixtures (Category 2), H252

Acute toxicity, Oral (Category 4), H302

Serious eye damage (Category 1), H318

Skin sensitisation (Category 1), H317

Acute aquatic toxicity (Category 3), H402

Chronic aquatic toxicity (Category 3), H412

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

2.2 GHS Label elements, including precautionary statements

Pictogram



Signal word : Danger

Hazard statement(s)

H252 : Self-heating in large quantities; may catch fire.
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 statement(s)

P235 + P410 : Keep cool. Protect from sunlight.

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/ protective clothing/ eye protection/ face protection.
P301 + P312	IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell.
P302 + P352	IF ON SKIN: Wash with plenty of soap and water.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P310	Immediately call a POISON CENTER/doctor.
P321	Specific treatment (see supplemental first aid instructions on this label).
P330	Rinse mouth.
P333 + P313	If skin irritation or rash occurs: Get medical advice/ attention.
P363	Wash contaminated clothing before reuse.
P407	Maintain air gap between stacks/ pallets.
P410	Protect from sunlight.
P413	Store bulk masses greater than .? kg/ .? lbs at temperatures not exceeding .? °C/ .? °F.
P420	Store away from other materials.
P501	Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms	:	1-Chloromethyl-4-fluoro-1,4-diazoniabicyclo[2.2.2]octane bis(tetrafluoroborate) N-Chloromethyl-N'-fluorotriethylenediammonium bis(tetrafluoroborate) F-TEDA
Formula	:	C ₇ H ₁₄ B ₂ ClF ₉ N ₂
Molecular weight	:	354.26 g/mol
CAS-No.	:	140681-55-6
Index-No.	:	005-015-00-6

Hazardous components

Component	Classification	Concentration
1,4-Diazoniabicyclo[2.2.2]octane, 1-(chloromethyl)-4-fluoro-, tetrafluoroborate(1-) (1:2)		
	Self-heat. 2; Acute Tox. 4; Eye Dam. 1; Skin Sens. 1; Aquatic Acute 3; Aquatic Chronic 3; H252, H302, H317, H318, H412	<= 100 %

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

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. 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.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Consult a physician. First treatment with calcium gluconate paste.

In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

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

5. FIREFIGHTING MEASURES

5.1 Extinguishing media

Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture

No data available

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information

Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust.

For personal protection see section 8.

6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up

Sweep up and shovel. Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13). Keep in suitable, closed containers for disposal. Contain spillage, pick up with an electrically protected vacuum cleaner or by wet-brushing and transfer to a container for disposal according to local regulations (see section 13).

6.4 Reference to other sections

For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid formation of dust and aerosols.

Provide appropriate exhaust ventilation at places where dust is formed. Keep away from sources of ignition - No smoking.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place.

Recommended storage temperature 2 - 8 °C

Handle and store under inert gas. Keep in a dry place.

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters

Contains no substances with occupational exposure limit values.

8.2 Exposure controls

Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye/face protection

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: Dermatrill® (KCL 740 / Aldrich Z677272, Size M)

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: Dermatrill® (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face particle respirator type N100 (US) or type P3 (EN 143) respirator cartridges as a backup to engineering controls. If the respirator is the

sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

- | | |
|---|---|
| a) Appearance | Form: powder
Colour: white |
| b) Odour | No data available |
| c) Odour Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | Melting point/range: 260 °C (500 °F) - lit. |
| f) Initial boiling point and boiling range | No data available |
| g) Flash point | No data available |
| h) Evaporation rate | No data available |
| i) Flammability (solid, gas) | No data available |
| j) Upper/lower flammability or explosive limits | No data available |
| k) Vapour pressure | No data available |
| l) Vapour density | No data available |
| m) Relative density | No data available |
| n) Water solubility | soluble |
| o) Partition coefficient: n-octanol/water | No data available |
| p) Auto-ignition temperature | The substance or mixture is classified as self heating with the category 2. |
| q) Decomposition temperature | No data available |
| r) Viscosity | No data available |
| s) Explosive properties | No data available |
| t) Oxidizing properties | No data available |

9.2 Other safety information

No data available

10. STABILITY AND REACTIVITY

10.1 Reactivity

No data available

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

Avoid moisture.

10.5 Incompatible materials

Strong oxidizing agents

10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NOx), Hydrogen chloride gas, Hydrogen fluoride, Borane/boron oxides

Other decomposition products - Gaseous hydrogen fluoride (HF).

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

LD50 Dermal - Rat - > 2,000 mg/kg

No data available

Skin corrosion/irritation

Serious eye damage/eye irritation

Severe eye irritation

Respiratory or skin sensitisation

Germ cell mutagenicity

No data available

Carcinogenicity

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

NTP: No component 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 identified as a carcinogen or potential carcinogen by OSHA.

Reproductive toxicity

No data available

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

Additional Information

RTECS: Not available

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

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to fish LC50 - Oncorhynchus mykiss (rainbow trout) - 100.0 mg/l - 24.0 h

Toxicity to daphnia and other aquatic invertebrates EC50 - Daphnia magna (Water flea) - 25 mg/l - 48 h

12.2 Persistence and degradability

12.3 Bioaccumulative potential

No data available

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 Other adverse effects

Harmful to aquatic life.

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product

Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

Contaminated packaging

Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)

UN number: 3088 Class: 4.2 Packing group: II

Proper shipping name: Self-heating solid, organic, n.o.s. (1,4-Diazoniabicyclo[2.2.2]octane, 1-(chloromethyl)-4-fluoro-, tetrafluoroborate(1-) (1:2))

Reportable Quantity (RQ):

Poison Inhalation Hazard: No

IMDG

UN number: 3088 Class: 4.2 Packing group: II EMS-No: F-A, S-J

Proper shipping name: SELF-HEATING SOLID, ORGANIC, N.O.S. (1,4-Diazoniabicyclo[2.2.2]octane, 1-(chloromethyl)-4-fluoro-, tetrafluoroborate(1-) (1:2))

IATA

UN number: 3088 Class: 4.2 Packing group: II

Proper shipping name: Self-heating solid, organic, n.o.s. (1,4-Diazoniabicyclo[2.2.2]octane, 1-(chloromethyl)-4-fluoro-, tetrafluoroborate(1-) (1:2))

15. REGULATORY INFORMATION

SARA 302 Components

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

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

Reactivity Hazard, Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

No components are subject to the Massachusetts Right to Know Act.

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
1,4-Diazoniabicyclo[2.2.2]octane, 1-(chloromethyl)-4-fluoro-, tetrafluoroborate(1-) (1:2)	140681-55-6	

New Jersey Right To Know Components

	CAS-No.	Revision Date
1,4-Diazoniabicyclo[2.2.2]octane, 1-(chloromethyl)-4-fluoro-, tetrafluoroborate(1-) (1:2)	140681-55-6	

California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION**Full text of H-Statements referred to under sections 2 and 3.**

Acute Tox.	Acute toxicity
Aquatic Acute	Acute aquatic toxicity
Aquatic Chronic	Chronic aquatic toxicity
Eye Dam.	Serious eye damage
H252	Self-heating in large quantities; may catch fire.
H302	Harmful if swallowed.
H317	May cause an allergic skin reaction.
H318	Causes serious eye damage.
H402	Harmful to aquatic life.
H412	Harmful to aquatic life with long lasting effects.

HMIS Rating

Health hazard:	2
Chronic Health Hazard:	*
Flammability:	0
Physical Hazard	2

NFPA Rating

Health hazard:	2
Fire Hazard:	0
Reactivity Hazard:	2

Further information

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Preparation Information

Sigma-Aldrich Corporation
 Product Safety – Americas Region
 1-800-521-8956

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