

## SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Version 5.2 Revision Date 17.01.2014

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

#### 1.1 Product identifiers

Product name : Selectfluor® fluorinating reagent

Product Number : 439479

Brand : Aldrich

Index-No. : 005-015-00-6

REACH No. : A registration number is not available for this substance as the substance or its uses are exempted from registration, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

CAS-No. : 140681-55-6

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

Identified uses : Laboratory chemicals, Manufacture of substances

#### 1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Company Ltd.  
The Old Brickyard  
NEW ROAD, GILLINGHAM  
Dorset  
SP8 4XT  
UNITED KINGDOM

Telephone : +44 (0)1747 833000

Fax : +44 (0)1747 833313

E-mail address : eurtechserv@sial.com

#### 1.4 Emergency telephone number

Emergency Phone # : +44 (0)1747 833100

### SECTION 2: Hazards identification

#### 2.1 Classification of the substance or mixture

##### Classification according to Regulation (EC) No 1272/2008

Self-heating substances (Category 2), H252

Acute toxicity, Oral (Category 4), H302

Serious eye damage (Category 1), H318

Skin sensitisation (Category 1), H317

Chronic aquatic toxicity (Category 3), H412

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

##### Classification according to EU Directives 67/548/EEC or 1999/45/EC

Xn	Harmful	R22
Xi	Irritant	R41
		R43
		R52/53

For the full text of the R-phrases mentioned in this Section, see Section 16.

#### 2.2 Label elements

##### Labelling according Regulation (EC) No 1272/2008

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.

P273

Avoid release to the environment.

P280

Wear protective gloves/ eye protection/ face protection.

P305 + P351 + P338

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

Supplemental Hazard  
Statements

none

### 2.3 Other hazards - none

## SECTION 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 :  $C_7H_{14}B_2ClF_9N_2$

Molecular Weight : 354.26 g/mol

CAS-No. : 140681-55-6

Index-No. : 005-015-00-6

#### Hazardous ingredients according to Regulation (EC) No 1272/2008

Component		Classification	Concentration
<b>1,4-Diazoniabicyclo[2.2.2]octane, 1-(chloromethyl)-4-fluoro-, tetrafluoroborate(1-) (1:2)</b>			
CAS-No.	140681-55-6	Self-heat. 2; Acute Tox. 4; Eye Dam. 1; Skin Sens. 1; Aquatic Chronic 3; H252, H302, H317, H318, H412	<= 100 %
Index-No.	005-015-00-6		

#### Hazardous ingredients according to Directive 1999/45/EC

Component		Classification	Concentration
<b>1,4-Diazoniabicyclo[2.2.2]octane, 1-(chloromethyl)-4-fluoro-, tetrafluoroborate(1-) (1:2)</b>			
CAS-No.	140681-55-6	Xn, R22 - R41 - R43 - R52/53	<= 100 %
Index-No.	005-015-00-6		

For the full text of the H-Statements and R-Phrases mentioned in this Section, see Section 16

## SECTION 4: First aid measures

### 4.1 Description of first aid measures

#### General advice

Consult a physician. Show this safety data sheet to the doctor in attendance.

#### 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.

**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

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**SECTION 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**

Carbon oxides, nitrogen oxides (NOx), Hydrogen chloride gas, Hydrogen fluoride, Borane/boron oxides

**5.3 Advice for firefighters**

Wear self contained breathing apparatus for fire fighting if necessary.

**5.4 Further information**

Use water spray to cool unopened containers.

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**SECTION 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.

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**SECTION 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**

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

Recommended storage temperature: 2 - 8 °C

Handle and store under inert gas.

### 7.3 Specific end use(s)

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

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## SECTION 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.

The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

##### Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

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

##### Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested:Dermatril® (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.

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## SECTION 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 - 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

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## SECTION 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

Other decomposition products - no data available

In the event of fire: see section 5

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## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - rat - 500 mg/kg

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

#### 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.

#### 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

#### Additional Information

RTECS: Not available

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

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## SECTION 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.

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## SECTION 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.

#### Contaminated packaging

Dispose of as unused product.

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## SECTION 14: Transport information

### 14.1 UN number

ADR/RID: 3088

IMDG: 3088

IATA: 3088

### 14.2 UN proper shipping name

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

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

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

### 14.3 Transport hazard class(es)

ADR/RID: 4.2

IMDG: 4.2

IATA: 4.2

### 14.4 Packaging group

ADR/RID: II

IMDG: II

IATA: II

### 14.5 Environmental hazards

ADR/RID: no

IMDG Marine pollutant: no

IATA: no

### 14.6 Special precautions for user

no data available

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## SECTION 15: Regulatory information

This safety datasheet complies with the requirements of Regulation (EC) No. 1907/2006.

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

no data available

### 15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out

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## SECTION 16: Other information

### Full text of H-Statements referred to under sections 2 and 3.

Acute Tox.	Acute 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.
H412	Harmful to aquatic life with long lasting effects.
Self-heat.	Self-heating substances
Skin Sens.	Skin sensitisation

**Full text of R-phrases referred to under sections 2 and 3**

Xn	Harmful
R22	Harmful if swallowed.
R41	Risk of serious damage to eyes.
R43	May cause sensitisation by skin contact.
R52/53	Harmful to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

**Further information**

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