

# SAFETY DATA SHEET

Version 6.6  
Revision Date 09/08/2024  
Print Date 09/09/2024

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

### 1.1 Product identifiers

Product name : Xenon difluoride  
Product Number : 394505  
Brand : Aldrich  
CAS-No. : 13709-36-9

### 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

### 2.1 Classification of the substance or mixture

#### GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Oxidizing solids (Category 2), H272  
Acute toxicity, Oral (Category 3), H301  
Acute toxicity, Inhalation (Category 1), H330  
Skin corrosion (Category 1B), H314

Serious eye damage (Category 1), H318

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 Statements

H272

May intensify fire; oxidizer.

H301

Toxic if swallowed.

H314

Causes severe skin burns and eye damage.

H330

Fatal if inhaled.

Precautionary Statements

P210

Keep away from heat.

P220

Keep/Store away from clothing/ combustible materials.

P221

Take any precaution to avoid mixing with combustibles.

P260

Do not breathe dust/ fume/ gas/ mist/ vapors/ spray.

P264

Wash skin thoroughly after handling.

P270

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

P271

Use only outdoors or in a well-ventilated area.

P280

Wear protective gloves/ protective clothing/ eye protection/ face protection.

P284

Wear respiratory protection.

P301 + P310 + P330

IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth.

P301 + P330 + P331

IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

P303 + P361 + P353

IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.

P304 + P340 + P310

IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.

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.

P363

Wash contaminated clothing before reuse.

P370 + P378

In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.

P403 + P233

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

P405

Store locked up.

P501

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

## 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS

Strong hydrogen fluoride-releaser

---

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Formula : F<sub>2</sub>Xe

Aldrich - 394505

Page 2 of 11

Molecular weight : 169.29 g/mol  
 CAS-No. : 13709-36-9  
 EC-No. : 237-251-2

Component	Classification	Concentration
<b>xenon difluoride</b>		
	Ox. Sol. 2; Acute Tox. 3; Acute Tox. 1; Skin Corr. 1B; Eye Dam. 1; H272, H301, H330, H314, H318	<= 100 %

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

If swallowed: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only in persons who are wide awake and fully conscious), administer activated charcoal (20 - 40 g in a 10% slurry) and consult a doctor as quickly as possible. 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**

Use extinguishing measures that are appropriate to local circumstances and the surrounding environment.

##### **Unsuitable extinguishing media**

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

#### **5.2 Special hazards arising from the substance or mixture**

Hydrogen fluoride

Not combustible.

Has a fire-promoting effect due to release of oxygen.

Ambient fire may liberate hazardous vapours.

#### **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**

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: Avoid generation and inhalation of dusts in all circumstances. Avoid substance contact. Ensure adequate ventilation. 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.

#### **6.3 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 carefully. Dispose of properly. Clean up affected area. Avoid generation of dusts.

#### **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.

#### Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition.

#### 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

Tightly closed. Keep locked up or in an area accessible only to qualified or authorized persons. Do not store near combustible materials.

Moisture sensitive. Handle under nitrogen, protect from moisture. Store under nitrogen. Do not store in glass

#### Storage class

Storage class (TRGS 510): 5.1B: Oxidizing hazardous materials

### 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

Component	CAS-No.	Value	Control parameters	Basis
xenon difluoride	13709-36-9	TWA	2.5 mg/m <sup>3</sup>	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		TWA	2.5 mg/m <sup>3</sup>	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Not classifiable as a human carcinogen		

		PEL	2.5 mg/m <sup>3</sup>	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
--	--	-----	-----------------------	---

### Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis
xenon difluoride	13709-36-9	Fluoride	2 mg/l	Urine	ACGIH - Biological Exposure Indices (BEI)
	Remarks	Prior to shift (16 hours after exposure ceases)			
		Fluoride	3 mg/l	Urine	ACGIH - Biological Exposure Indices (BEI)
		End of shift (As soon as possible after exposure ceases)			

## 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 EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested:KCL 741 Dermatril® L

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](http://www.kcl.de)).

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested:KCL 741 Dermatril® L

### **Body Protection**

protective clothing

### **Respiratory protection**

Recommended Filter type: Filter type P3

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 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.

### **Control of environmental exposure**

Do not let product enter drains.

---

## **SECTION 9: Physical and chemical properties**

### **9.1 Information on basic physical and chemical properties**

a) Appearance	Form: solid
b) Odor	No data available
c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/ range: 129 °C (264 °F) - lit.
f) Initial boiling point and boiling range	No data available
g) Flash point	( )Not applicable
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	No data available
k) Vapor pressure	3.8 hPa at 25 °C (77 °F)
l) Vapor density	No data available
m) Density	4.32 g/mL at 25 °C (77 °F) - lit.
Relative density	No data available
n) Water solubility	(decomposition)
o) Partition coefficient: n-octanol/water	No data available
p) Autoignition temperature	No data available

Aldrich - 394505

Page 7 of 11

- q) Decomposition temperature > 800 °C (> 1472 °F) -
- r) Viscosity No data available
- s) Explosive properties No data available
- t) Oxidizing properties The substance or mixture is classified as oxidizing with the category 2.

## 9.2 Other safety information

No data available

---

## SECTION 10: Stability and reactivity

### 10.1 Reactivity

No data available

### 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:

Acetone

powdered aluminium

combustible substances

magnesium

Organic Substances

Exothermic reaction with:

Reducing agents

### 10.4 Conditions to avoid

Reacts dangerously with glass.

no information available

### 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 - Mouse - 90 mg/kg

Remarks: (RTECS)

LC50 Inhalation - 4 h - 0.005 mg/l - dust/mist

Dermal: No data available

No data available

Aldrich - 394505

Page 8 of 11



**Skin corrosion/irritation**

Remarks: No data available

**Serious eye damage/eye irritation**

Remarks: No data available

**Respiratory or skin sensitization**

No data available

**Germ cell mutagenicity**

No data available

**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**

RTECS: ZE1294166

Fluoride ion can reduce serum calcium levels possibly causing fatal hypocalcemia.

Cough, Shortness of breath, Headache, Nausea, Vomiting

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

---

**SECTION 12: Ecological information****12.1 Toxicity**

No data available

**12.2 Persistence and degradability**

No data available

**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 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: 3087 Class: 5.1 (6.1) Packing group: II  
Proper shipping name: Oxidizing solid, toxic, n.o.s. (xenon difluoride)  
Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

### IMDG

UN number: 3087 Class: 5.1 (6.1) Packing group: II EMS-No: F-A, S-Q  
Proper shipping name: OXIDIZING SOLID, TOXIC, N.O.S. (xenon difluoride)

### IATA

UN number: 3087 Class: 5.1 (6.1) Packing group: II  
Proper shipping name: Oxidizing solid, toxic, n.o.s. (xenon difluoride)

---

## 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

**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.

#### **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

### **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**

### **Further 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](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact [mlsbranding@sial.com](mailto:mlsbranding@sial.com).

Version: 6.6

Revision Date: 09/08/2024

Print Date: 09/09/2024