

SAFETY DATA SHEET

Version 4.2
Revision Date 07/03/2014
Print Date 10/23/2019

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

Product name : Hexafluoroacetone deuterate

Product Number : 534773
Brand : Aldrich

CAS-No. : 72301-81-6

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
3050 Spruce Street
SAINT LOUIS MO 63103
USA

Telephone : +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)**

Acute toxicity, Oral (Category 3), H301
Acute toxicity, Inhalation (Category 3), H331
Acute toxicity, Dermal (Category 3), H311
Skin irritation (Category 2), H315
Eye irritation (Category 2A), H319
Reproductive toxicity (Category 1B), H360
Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335

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)

H301 + H311 + H331

H315

H319

H335

H360

Toxic if swallowed, in contact with skin or if inhaled
Causes skin irritation.
Causes serious eye irritation.
May cause respiratory irritation.
May damage fertility or the unborn child.

Precautionary statement(s)

P201

P202

Obtain special instructions before use.
Do not handle until all safety precautions have been read and

P261	understood.
P264	Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
P270	Wash skin thoroughly after handling.
P271	Do not eat, drink or smoke when using this product.
P280	Use only outdoors or in a well-ventilated area.
P301 + P310	Wear protective gloves/ eye protection/ face protection.
P302 + P352	IF SWALLOWED: Immediately call a POISON CENTER or doctor/ physician.
P304 + P340	IF ON SKIN: Wash with plenty of soap and water.
P305 + P351 + P338	IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
P308 + P313	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P322	IF exposed or concerned: Get medical advice/ attention.
P330	Specific measures (see supplemental first aid instructions on this label).
P332 + P313	Rinse mouth.
P337 + P313	If skin irritation occurs: Get medical advice/ attention.
P361	If eye irritation persists: Get medical advice/ attention.
P403 + P233	Remove/Take off immediately all contaminated clothing.
P405	Store in a well-ventilated place. Keep container tightly closed.
P501	Store locked up.
	Dispose of contents/ container to an approved waste disposal plant.

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

Reacts violently with water.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms : Hexafluoro-2-propanone deuterate

Formula : $C_3F_6O \cdot D_2O$

Molecular Weight : 186.05 g/mol

CAS-No. : 72301-81-6

Hazardous components

Component	Classification	Concentration
Hexafluoroacetone deuterate		
	Acute Tox. 3; Skin Irrit. 2; Eye Irrit. 2A; Repr. 1B; STOT SE 3; H301 + H311 + H331, H315, H319, H335, H360	-

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

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

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. Take victim immediately to hospital. 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

5. FIREFIGHTING MEASURES

5.1 Extinguishing media

Suitable extinguishing media

Dry powder

5.2 Special hazards arising from the substance or mixture

Carbon oxides, Hydrogen fluoride

5.3 Advice for firefighters

Wear self contained breathing apparatus for fire fighting if necessary.

5.4 Further information

no data available

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Wear respiratory protection. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas.

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.

6.3 Methods and materials for containment and cleaning up

Soak up with inert absorbent material and dispose of as hazardous waste. Do not flush with water. Keep in suitable, closed containers for disposal.

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 inhalation of vapour or mist.

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. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Never allow product to get in contact with water during storage.

Store under inert gas. Hygroscopic.

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

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

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.

Body Protection

Complete suit protecting against chemicals, Flame retardant protective clothing, 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 respirator with multi-purpose combination (US) or type ABEK (EN 14387) 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.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a) Appearance	Form: liquid Colour: colourless
b) Odour	no data available
c) Odour Threshold	no data available
d) pH	no data available
e) Melting point/freezing point	Melting point/range: -129 °C (-200 °F)
f) Initial boiling point and boiling range	104 - 108 °C (219 - 226 °F) - lit.
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	6.7 hPa (5.0 mmHg) at 25 °C (77 °F)
l) Vapour density	5.73 - (Air = 1.0)
m) Relative density	1.579 g/cm ³
n) Water solubility	no data available
o) Partition coefficient: n-octanol/water	no data available
p) Auto-ignition temperature	no data available
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

Relative vapour density 5.73 - (Air = 1.0)

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

Reacts violently with water.

10.4 Conditions to avoid

Exposure to moisture.

10.5 Incompatible materials

Strong oxidizing agents
Reacts violently with water., Strong oxidizing agents

10.6 Hazardous decomposition products

Other decomposition products - no data available
In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

no data available

no data available

Skin corrosion/irritation

no data available

Serious eye damage/eye irritation

no data available

Respiratory or skin sensitisation

no data available

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

Presumed human reproductive toxicant

no data available

Specific target organ toxicity - single exposure

Inhalation - May cause respiratory irritation.

Specific target organ toxicity - repeated exposure

no data available

Aspiration hazard

no data available

Additional Information

RTECS: Not available

burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea, Vomiting, Dizziness, Central nervous system depression

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

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 Other adverse effects

no data available

13. DISPOSAL CONSIDERATIONS**13.1 Waste treatment methods****Product**

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: 2552 Class: 6.1 Packing group: II

Proper shipping name: Hexafluoroacetone hydrate, liquid

Marine pollutant: No

Poison Inhalation Hazard: No

IMDG

UN number: 2552 Class: 6.1 Packing group: II EMS-No: F-A, S-A

Proper shipping name: HEXAFLUOROACETONE HYDRATE, LIQUID

Marine pollutant: No

IATA

UN number: 2552 Class: 6.1 Packing group: II

Proper shipping name: Hexafluoroacetone hydrate, liquid

15. REGULATORY INFORMATION**SARA 302 Components**

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

SARA 313 Components

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.

SARA 311/312 Hazards

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
Hexafluoroacetone deuterate	72301-81-6	

New Jersey Right To Know Components

	CAS-No.	Revision Date
Hexafluoroacetone deuterate	72301-81-6	

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
Eye Irrit.	Eye irritation
H301	Toxic if swallowed.
H301 + H311 + H331	Toxic if swallowed, in contact with skin or if inhaled
H311	Toxic in contact with skin.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H331	Toxic if inhaled.
H335	May cause respiratory irritation.

HMIS Rating

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

NFPA Rating

Health hazard:	4
Fire Hazard:	0
Reactivity Hazard:	0

Further information

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Preparation Information

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

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