

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name : Hexafluoroacetone trihydrate

Product Number : 139238
Brand : Aldrich

CAS-No. : 34202-69-2

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 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 2), H310
Skin corrosion (Category 1B), H314
Serious eye damage (Category 1), H318
Reproductive toxicity (Category 2), H361

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 + H331 : Toxic if swallowed or if inhaled
H310 : Fatal in contact with skin.
H314 : Causes severe skin burns and eye damage.
H318 : Causes serious eye damage.
H361 : Suspected of damaging fertility or the unborn child.

Precautionary statement(s)

P201 : Obtain special instructions before use.
P202 : Do not handle until all safety precautions have been read and

P261	understood.
P262	Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
P264	Do not get in eyes, on skin, or on clothing.
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.
P281	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P310 + P330	Use personal protective equipment as required. 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): Remove/ Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P310	IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing. Immediately call a POISON CENTER or doctor/ physician.
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.
P308 + P313	IF exposed or concerned: Get medical advice/ attention.
P363	Wash contaminated clothing before reuse.
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 - none

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms	:	Perfluoroacetone trihydrate Hexafluoro-2-propanone trihydrate
Formula	:	C ₃ F ₆ O · 3H ₂ O
Molecular weight	:	220.07 g/mol
CAS-No.	:	34202-69-2
EC-No.	:	211-676-3

Hazardous components

Component	Classification	Concentration
Hexafluoroacetone trihydrate		
	Acute Tox. 3; Acute Tox. 2; Skin Corr. 1B; Eye Dam. 1; Repr. 2; H301 + H331, H310, H314, H361	<= 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

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

Take off contaminated clothing and shoes immediately. 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. Continue rinsing eyes during transport to hospital.

If swallowed

Do NOT induce vomiting. 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

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. 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.

Moisture sensitive.

Storage class (TRGS 510): Non-combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials

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**

Component	CAS-No.	Value	Control parameters	Basis
Hexafluoroacetone trihydrate	34202-69-2	TWA	0.100000 ppm 0.700000 mg/m3	USA. NIOSH Recommended Exposure Limits
	Remarks	Potential for dermal absorption		
		PEL	0.1 ppm 0.7 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		

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

Tightly fitting safety goggles. Faceshield (8-inch minimum). 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, 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: 18 - 21 °C (64 - 70 °F) - lit. |
| f) Initial boiling point and boiling range | 106 - 108 °C (223 - 226 °F) at 1,013 hPa (760 mmHg) |
| 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 | 14,681.6 hPa (11,012.1 mmHg) at 55 °C (131 °F)
6,031.2 hPa (4,523.8 mmHg) at 21 °C (70 °F) |

l) Vapour density	7.6 - (Air = 1.0)
m) Relative density	1.579 g/cm ³ at 25 °C (77 °F)
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 7.6 - (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

No data available

10.4 Conditions to avoid

Do not allow water to enter container.

10.5 Incompatible materials

Reacts violently with water., Strong oxidizing agents

10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Hydrogen fluoride
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

LD50 Oral - Rat - 190 mg/kg

Remarks: Behavioral:Somnolence (general depressed activity).

LD50 Dermal - Rabbit - 113 mg/kg

Remarks: Behavioral:Somnolence (general depressed activity). Skin irritation

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.
- 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

Possible risk of congenital malformation in the fetus.

Suspected human reproductive toxicant

No data available

Reproductive toxicity - Rat - Skin

Effects on Fertility: Litter size (e.g.; # fetuses per litter; measured before birth). Effects on Embryo or Fetus: Fetal death.

Specific Developmental Abnormalities: Craniofacial (including nose and tongue).

No data available

Developmental Toxicity - Rat - Skin

Specific Developmental Abnormalities: Central nervous system. Specific Developmental Abnormalities: Eye, ear.

Developmental Toxicity - Rat - Skin

Specific Developmental Abnormalities: Urogenital system.

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: UC2700000

Cough, Shortness of breath, Headache, Nausea, Vomiting, Dizziness, Central nervous system depression

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

Reportable Quantity (RQ):

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

IATA

UN number: 2552 Class: 6.1 Packing group: II

Proper shipping name: Hexafluoroacetone hydrate, liquid

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

Sudden Release of Pressure Hazard, Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

	CAS-No.	Revision Date
Hexafluoroacetone trihydrate	34202-69-2	1991-07-01

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Hexafluoroacetone trihydrate	34202-69-2	1991-07-01

New Jersey Right To Know Components

	CAS-No.	Revision Date
Hexafluoroacetone trihydrate	34202-69-2	1991-07-01

California Prop. 65 Components

	CAS-No.	Revision Date
WARNING: This product contains a chemical known to the State of California to cause birth defects or other reproductive harm.	34202-69-2	2014-06-06

Hexafluoroacetone trihydrate

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

Acute Tox.	Acute toxicity
Eye Dam.	Serious eye damage
H301	Toxic if swallowed.
H301 + H331	Toxic if swallowed or if inhaled
H310	Fatal in contact with skin.
H314	Causes severe skin burns and eye damage.
H318	Causes serious eye damage.
H331	Toxic if inhaled.

H361 Suspected of damaging fertility or the unborn child.

HMIS Rating

Health hazard: 4
Chronic Health Hazard: *
Flammability: 1
Physical Hazard 1

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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