

• SAFETY DATA SHEET

Version 6.11
Revision Date 01/20/2026
Print Date 01/21/2026

SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : 1,1,1,3,3,3-Hexafluoro-2-propanol-d2
Product Number : 440671
Brand : Aldrich
CAS-No. : 38701-74-5

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 number

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2. HAZARDS IDENTIFICATION

GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

Hazards for the product as supplied


Skin corrosion : Sub-category 1A

Serious eye damage : Category 1
Reproductive toxicity : Category 2
Specific target organ toxicity - repeated exposure (Oral) : Category 2 (Central nervous system)

Other hazards

None known.

GHS label elements

Hazard pictograms : 

Signal word : Danger

Hazard statements : H314 Causes severe skin burns and eye damage.
H361 Suspected of damaging fertility or the unborn child.
H373 May cause damage to organs (Central nervous system) through prolonged or repeated exposure if swallowed.

Precautionary statements : **Prevention:**
P201 Obtain special instructions before use.
P202 Do not handle until all safety precautions have been read and understood.
P260 Do not breathe mist or vapours.
P264 Wash skin thoroughly after handling.
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.

Response:

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.
P308 + P313 IF exposed or concerned: Get medical advice/ attention.
P363 Wash contaminated clothing before reuse.

Storage:

P405 Store locked up.

Disposal:

P501 Dispose of contents/ container to an approved waste disposal plant.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

CAS-No. : 38701-74-5

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
1,1,1,3,3,3-hexafluoro[2- ² H]propan-2-[² H]ol	38701-74-5*	>= 80 - <= 100	TSC

* Indicates that the identifier is a CAS No.

TSC- the actual concentration or concentration range is withheld as a trade secret

SECTION 4. FIRST AID MEASURES

- General advice : First aiders need to protect themselves. Show this safety data sheet to the doctor in attendance.
- If inhaled : After inhalation: fresh air. Call in physician.
- In case of skin contact : 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 : After swallowing: make victim drink water (two glasses at most), avoid vomiting (risk of perforation). Call a physician immediately. Do not attempt to neutralise.
- 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
- Protection of first-aiders : For personal protection see section 8.

Notes to physician : No data available

SECTION 5. FIREFIGHTING MEASURES

- Suitable extinguishing media : Foam
Carbon dioxide (CO₂)
Dry powder
- Unsuitable extinguishing media : For this substance/mixture no limitations of extinguishing agents are given.
- Specific hazards during fire fighting : Combustible.

Development of hazardous combustion gases or vapours possible in the event of fire.
- Hazardous combustion products : Carbon oxides

Hydrogen fluoride
- Specific extinguishing methods : No data available
- Further information : Suppress (knock down) gases/vapours/mists with a water spray jet.
Prevent fire extinguishing water from contaminating surface water or the ground water system.
- Special protective equipment for fire-fighters : Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

SECTION 6. ACCIDENTAL RELEASE MEASURES

- Personal precautions, protective equipment and emergency procedures : Advice for non-emergency personnel:
Do not breathe vapours, aerosols.
Avoid substance contact.
Ensure adequate ventilation.
Evacuate the danger area, observe emergency procedures, consult an expert.
Advice for emergency responders:

For personal protection see section 8.

Environmental precautions : Do not let product enter drains.

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 with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

Further information on storage conditions : Tightly closed.

Storage class : 8A, Combustible, corrosive hazardous materials

Recommended storage temperature : Recommended storage temperature see product label.

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

Engineering measures : No data available

Personal protective equipment

Respiratory protection : required when vapours/aerosols 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.

Recommended Filter type: : Filter type AX

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.

- Hand protection
- Material : Viton®
 - Break through time : 480 min
 - Glove thickness : 0.7 mm
 - Protective index : Full contact
 - Manufacturer : Vitoject® (KCL 890 / Aldrich Z677698, Size M)

 - Material : Nitrile rubber
 - Break through time : 120 min
 - Glove thickness : 0.4 mm
 - Protective index : Splash contact
 - Manufacturer : Camatril® (KCL 730 / Aldrich Z677442, Size M)

 - Remarks : 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).
- Eye 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 and body protection : protective clothing
- Hygiene measures : Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

- Appearance : liquid

- Color : No data available

- Odor : No data available

- Odor Threshold : No data available
- pH : No data available

- Melting point/ range : 25 °F / -4 °C

- Boiling point/boiling range : 138 °F / 59 °C (1,013 hPa)

Flash point	: No data available
Evaporation rate	: No data available
Flammability (solid, gas)	: No data available
Flammability (liquids)	: No data available
Burning rate	: No data available
Upper explosion limit / Upper flammability limit	: No data available
Lower explosion limit / Lower flammability limit	: No data available
Vapor pressure	: No data available
Relative vapour density	: No data available
Relative density	: No data available
Density	: No data available
Water solubility	: No data available
Partition coefficient: n- octanol/water	: No data available
Autoignition temperature	: No data available
Decomposition temperature	: No data available
Viscosity, dynamic	: No data available
Viscosity, kinematic	: No data available
Flow time	: No data available
Explosive properties	: Not classified as explosive.
Oxidizing properties	: none
Molecular weight	: 170.03 g/mol
Particle characteristics Particle size	: No data available

SECTION 10. STABILITY AND REACTIVITY

Reactivity	: No data available
Chemical stability	: The product is chemically stable under standard ambient conditions (room temperature) .
Possibility of hazardous reactions	: Avoid moisture. Violent reactions possible with: Strong oxidizing agents Metals
Conditions to avoid	: no information available
Incompatible materials	: No data available
Hazardous decomposition products	: In the event of fire: see section 5

SECTION 11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

Oral: No data available

Inhalation: No data available

Dermal: No data available

Skin corrosion/irritation

Skin - Rabbit

Result: Corrosive

Remarks: (ECHA)

The value is given in analogy to the following substances: 1,1,1,3,3,3-hexafluoro-2-propanol

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Causes serious eye damage.

Remarks: (ECHA)

The value is given in analogy to the following substances: 1,1,1,3,3,3-hexafluoro-2-propanol

Remarks: Causes serious eye damage.

Respiratory or skin sensitization

Local lymph node assay (LLNA) - Mouse

Result: negative

(OECD Test Guideline 429)

Remarks: The value is given in analogy to the following substances: 1,1,1,3,3,3-hexafluoro-2-propanol

Germ cell mutagenicity

Test Type: Ames test

Test system: Escherichia coli/Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Remarks: The value is given in analogy to the following substances: 1,1,1,3,3,3-hexafluoro-2-propanol **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 on OSHA's list of regulated carcinogens.

Reproductive toxicity

Suspected of damaging the unborn child.

Suspected of damaging fertility.

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

Oral - May cause damage to organs through prolonged or repeated exposure.

- Central nervous system

Remarks: The value is given in analogy to the following substances: 1,1,1,3,3,3-hexafluoro-2-propanol

Aspiration hazard

No data available

11.2 Additional Information

Repeated dose toxicity - Rat - male and female - Oral - 42 Days - No observed adverse effect level - 60 mg/kg - Lowest observed adverse effect level - 300 mg/kg

Remarks: The value is given in analogy to the following substances: 1,1,1,3,3,3-hexafluoro-2-propanol

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity

Components:

1,1,1,3,3,3-hexafluoro[2-²H]propan-2-[²H]ol:

Toxicity to fish : LC50 (Pimephales promelas (fathead minnow)): 244.0 mg/l

Exposure time: 96 h

Remarks: (ECOTOX Database)

The value is given in analogy to the following substances:

The value is given in analogy to the following substances: 1,1,1,3,3,3-hexafluoro-2-propanol

Toxicity to daphnia and : EC50 (Daphnia magna (Water flea)): > 97.3 mg/l

other aquatic
invertebrates

End point: Immobilization
Exposure time: 48 h
Test Type: static test
Analytical monitoring: yes
Method: OECD Test Guideline 202
GLP: yes
Remarks: The value is given in analogy to the
following substances:
The value is given in analogy to the following
substances: 1,1,1,3,3,3-hexafluoro-2-propanol

Toxicity to algae/aquatic
plants

: ErC50 (Pseudokirchneriella subcapitata (green
algae)): > 100 mg/l
Exposure time: 72 h
Test Type: static test
Analytical monitoring: yes
Method: OECD Test Guideline 201
GLP: yes
Remarks: The value is given in analogy to the
following substances:
The value is given in analogy to the following
substances: 1,1,1,3,3,3-hexafluoro-2-propanol

NOEC (Pseudokirchneriella subcapitata (green algae)):
>= 100 mg/l
Exposure time: 72 h
Test Type: static test
Analytical monitoring: yes
Method: OECD Test Guideline 201
GLP: yes
Remarks: The value is given in analogy to the
following substances:
The value is given in analogy to the following
substances: 1,1,1,3,3,3-hexafluoro-2-propanol

Ecotoxicology Assessment

Acute aquatic toxicity : This product has no known ecotoxicological effects.

Chronic aquatic toxicity : This product has no known ecotoxicological effects.

Persistence and degradability

Components:

1,1,1,3,3,3-hexafluoro[2-²H]propan-2-[²H]ol:

Biodegradability : aerobic
Inoculum: activated sludge
Concentration: 100 mg/l
Result: Not readily biodegradable.
Biodegradation: 0 - 5 %
Exposure time: 28 d

Method: OECD Test Guideline 301C
Remarks: The value is given in analogy to the following substances:
The value is given in analogy to the following substances: 1,1,1,3,3,3-hexafluoro-2-propanol

Bioaccumulative potential

Components:

1,1,1,3,3,3-hexafluoro[2-²H]propan-2-[²H]ol:

Bioaccumulation : Species: Cyprinus carpio (Carp)
Bioconcentration factor (BCF): 1.1 - 1.4
Exposure time: 42 d
Temperature: 77 °F / 25 °C
Concentration: 1 mg/l
Method: OECD Test Guideline 305
Remarks: The value is given in analogy to the following substances:
The value is given in analogy to the following substances: 1,1,1,3,3,3-hexafluoro-2-propanol

Mobility in soil

No data available

Other adverse effects

Product:

Ozone-Depletion Potential : Regulation: 40 CFR Protection of Environment; Part 82 Protection of Stratospheric Ozone - CAA Section 602 Class I Substances
Remarks: This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

SECTION 13. DISPOSAL CONSIDERATIONS

Disposal methods

Waste from residues : 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

International Regulations

IATA-DGR

UN/ID No. : UN 3265

Aldrich - 440671

Page 11 of 15

Proper shipping name : Corrosive liquid, acidic, organic, n.o.s.
(1,1,1,3,3,3-hexafluoro[2-²H]propan-2-[²H]ol)
Class : 8
Packing group : II
Labels : Class 8 - Corrosive substances
Packing instruction (cargo aircraft) : 855
Packing instruction (passenger aircraft) : 851

IMDG-Code

UN number : UN 3265
Proper shipping name : CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S.
(1,1,1,3,3,3-hexafluoro[2-²H]propan-2-[²H]ol)
Class : 8
Packing group : II
Labels : 8
EmS Code : F-A, S-B
Marine pollutant : no

Transport in bulk according to IMO instruments

Not applicable for product as supplied.

National Regulations

49 CFR Road

UN/ID/NA number : UN 3265
Proper shipping name : Corrosive liquid, acidic, organic, n.o.s.
(1,1,1,3,3,3-hexafluoro[2-²H]propan-2-[²H]ol)
Class : 8
Packing group : II
Labels : Class 8 - Corrosive substances
ERG Code : 153
Marine pollutant : no

Poison Inhalation Hazard : No

Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

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 : 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.

Clean Air Act

This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

This product does not contain any hazardous air pollutants (HAP), as defined by the U.S. Clean Air Act Section 112 (40 CFR 61).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 111 SOCOMI Intermediate or Final VOC's (40 CFR 60.489).

Clean Water Act

This product does not contain any Hazardous Substances listed under the U.S. CleanWater Act, Section 311, Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. CleanWater Act, Section 311, Table 117.3.

This product does not contain any toxic pollutants listed under the U.S. Clean Water Act Section 307

This product does not contain any priority pollutants related to the U.S. Clean Water Act

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 components of this product are reported in the following inventories:

TSCA : Product contains substance(s) not listed on 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

Full text of other abbreviations

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

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 and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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Details in analogy to the undeuterated compound.

Revision Date : 01/20/2026

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