

SAFETY DATA SHEET

according to the OSHA
Hazard Communication Standard

Version 6.11
Revision Date 07/14/2026
Print Date 07/15/2026

SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : Trifluoroacetic acid-d

Product Number : 152005
Brand : Aldrich
CAS-No. : 599-00-8

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

Identified uses : Laboratory chemicals, Synthesis of substances

Restrictions on use : Not Available

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

Acute toxicity : Category 4
(Inhalation)

Skin corrosion : Category 1A

Serious eye damage : Category 1

Long-term (chronic) aquatic hazard : Category 3

Other hazards

None known.

GHS label elements

Hazard pictograms :



Signal word : Danger

Hazard statements : H314 Causes severe skin burns and eye damage.
H332 Harmful if inhaled.
H412 Harmful to aquatic life with long lasting effects.

Precautionary statements : **Prevention:**
P261 Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
P264 Wash skin thoroughly after handling.
P271 Use only outdoors or in a well-ventilated area.
P273 Avoid release to the environment.
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.
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. : 599-00-8

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
trifluoroacetic [2H]acid	599-00-8*	>= 90 - <= 100	-

* Indicates that the identifier is a CAS No.

Actual concentration 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. Immediately call in physician.
If breathing stops: immediately apply artificial respiration, if necessary also oxygen.
- 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 GHS label elements) 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	: 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.
Specific hazards during fire fighting	: Not combustible.
	Ambient fire may liberate hazardous vapours.
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: Wear appropriate personal protective equipment, as indicated in 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 with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

SECTION 7. HANDLING AND STORAGE

For precautions see section 2 GHS label elements

Advice on safe handling : Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Further information on storage conditions : Tightly closed.

Storage class : 8A, Combustible, corrosive hazardous materials

Recommended storage temperature : Recommended storage temperature see product label.

Further information on storage stability : Store under inert gas. hygroscopic

Packaging material : Suitable material: Clear Glass Bottle/Jar

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 ABEK

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 : butyl-rubber
Break through time : 480 min
Glove thickness : 0.7 mm
Protective index : Full contact
Manufacturer : Butoject® (KCL 898)

Material : Latex gloves
Break through time : 30 min
Glove thickness : 0.6 mm
Protective index : Splash contact
Manufacturer : Lapren® (KCL 706 / Aldrich Z677558, 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

Colour : No data available

Odour : No data available

Odour Threshold : No data available
pH : No data available

Melting point	: No data available
Boiling point/boiling range	: 167 °F / 75 °C Method: lit.
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
Vapour pressure	: No data available
Relative vapour density	: No data available
Relative density	: No data available
Density	: 1.493 g/cm ³ (77 °F / 25 °C) Method: lit.
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	: No data available
Oxidizing properties	: No data available
Molecular weight	: 115.02 g/mol

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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 : Risk of explosion with:
lithium aluminium hydride
Exothermic reaction with:
alkalines
Generates dangerous gases or fumes in contact with:
acids

Conditions to avoid : Avoid moisture.

no information available

Incompatible materials : rubber
Metals

Hazardous decomposition products : In the event of fire: see section 5

SECTION 11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

Symptoms: Nausea, Vomiting, strong pain (risk of perforation!), If ingested, severe burns of the mouth and throat, as well as a danger of perforation of the oesophagus and the stomach.

LC50 Inhalation - Rat - 4 h - 10.01 mg/l - vapour

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

The value is given in analogy to the following substances: trifluoroacetic acid

Inhalation: Corrosive to respiratory system.

Symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages:, damage of respiratory tract, Inhalation may lead to the formation of oedemas in the respiratory tract.

Dermal: No data available

Skin corrosion/irritation

Skin - Rabbit

Result: Causes severe burns.

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

The value is given in analogy to the following substances: trifluoroacetic acid

Remarks: Necrosis

Causes poorly healing wounds.

Serious eye damage/eye irritation

Remarks: Causes serious eye damage.

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

Test Type: Ames test

Test system: 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: trifluoroacetic acid

Test Type: In vitro mammalian cell gene mutation test

Test system: mouse lymphoma cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 476

Result: negative

Remarks: The value is given in analogy to the following substances: trifluoroacetic acid

Test Type: Chromosome aberration test in vitro

Test system: Human lymphocytes

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 473

Result: negative

Remarks: The value is given in analogy to the following substances: trifluoroacetic acid

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

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

Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., spasm, inflammation and edema of the larynx, spasm, inflammation and edema of the bronchi, pneumonitis, pulmonary edema, burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea, Vomiting
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Damage to:

Kidney

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

Liver - Irregularities - Based on Human Evidence

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity

Components:

trifluoroacetic [2H]acid:

Toxicity to fish	: LC50 (Danio rerio (zebra fish)): > 999 mg/l End point: mortality Exposure time: 96 h Test Type: static test Analytical monitoring: yes Method: OECD Test Guideline 203 GLP: yes Remarks: The value is given in analogy to the following substances: The value is given in analogy to the following substances: trifluoroacetic acid
Toxicity to daphnia and other aquatic invertebrates	: EC50 (Daphnia magna (Water flea)): > 999 mg/l 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: trifluoroacetic acid
Toxicity to algae/aquatic plants	: ErC50 (Pseudokirchneriella subcapitata): 237.07 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:

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The value is given in analogy to the following substances: trifluoroacetic acid

- Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity) : NOEC (Daphnia magna (Water flea)): > 25 mg/l
End point: reproduction rate
Exposure time: 21 d
Test Type: semi-static test
Analytical monitoring: yes
Method: OECD Test Guideline 211
GLP: yes
Remarks: The value is given in analogy to the following substances:
The value is given in analogy to the following substances: trifluoroacetic acid
- Toxicity to microorganisms : EC50 (activated sludge): > 832 mg/l
Exposure time: 3 h
Method: OECD Test Guideline 209
GLP: yes
Remarks: The value is given in analogy to the following substances:
The value is given in analogy to the following substances: trifluoroacetic acid

Ecotoxicology Assessment

- Chronic aquatic toxicity : Harmful to aquatic life with long lasting effects.
The value is given in analogy to the following substances: trifluoroacetic acid

Persistence and degradability

Components:

trifluoroacetic [2H]acid:

- Biodegradability : aerobic
Inoculum: activated sludge
Concentration: 20 mg/l
Result: Not inherently biodegradable.
Biodegradation: 11 %
Exposure time: 127 d
Method: OECD Test Guideline 301D
GLP: yes
Remarks: The value is given in analogy to the following substances:
The value is given in analogy to the following substances: trifluoroacetic acid

Bioaccumulative potential

Components:

trifluoroacetic [2H]acid:

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Bioaccumulation : Remarks: No bioaccumulation is to be expected (log Pow <= 4).

Mobility in soil

No data available

Other adverse effects

Components:

trifluoroacetic [2H]acid:

Additional ecological information : Harmful effect due to pH shift.
Caustic even in diluted form.
Hazard for drinking water supplies.

Discharge into the environment must be avoided.

Endocrine disrupting properties

No data available

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 2699
Proper shipping name : Trifluoroacetic acid
Class : 8
Packing group : I
Labels : Class 8 - Corrosive substances
Packing instruction (cargo aircraft) : 854
Packing instruction (passenger aircraft) : 850

IMDG-Code

UN number : UN 2699
Proper shipping name : TRIFLUOROACETIC ACID

Class : 8
Packing group : I
Labels : 8
EmS Code : F-A, S-B

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Marine pollutant : no

Transport in bulk according to IMO instruments

Not applicable for product as supplied.

National Regulations

49 CFR

UN/ID/NA number : UN 2699
Proper shipping name : Trifluoroacetic acid

Class : 8

Packing group : I
Labels : Class 8 - Corrosive substances
ERG Code : 154
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.

US State Regulations

Massachusetts Right To Know

No components are subject to the Massachusetts Right to Know Act.

Massachusetts Right To Know

No components are subject to the Massachusetts Right to Know Act.

Pennsylvania Right To Know

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

New Jersey Right To Know

trifluoroacetic [2H]acid

599-00-8

The components of this product are reported in the following inventories:

US 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**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.

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US / EN