

SAFETY DATA SHEET

according to the OSHA
Hazard Communication Standard

Version 6.12
Revision Date 07/15/2026
Print Date 07/16/2026

SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : α,α,α -Trifluorotoluene

Product Number : 547948
Brand : Sigma-Aldrich
Index-No. : 602-056-00-7
CAS-No. : 98-08-8

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

Flammable liquids : Category 2

Specific target organ
toxicity - repeated : Category 2

exposure

Short-term (acute) aquatic hazard : Category 2

Long-term (chronic) aquatic hazard : Category 2

Other hazards

None known.

GHS label elements

Hazard pictograms : 

Signal word : Danger

Hazard statements : H225 Highly flammable liquid and vapour.
H373 May cause damage to organs through prolonged or repeated exposure.
H411 Toxic to aquatic life with long lasting effects.

Precautionary statements : **Prevention:**
P210 Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P233 Keep container tightly closed.
P240 Ground/bond container and receiving equipment.
P241 Use explosion-proof electrical/ ventilating/ lighting equipment.
P242 Use only non-sparking tools.
P243 Take precautionary measures against static discharge.
P260 Do not breathe mist or vapours.
P273 Avoid release to the environment.
P280 Wear protective gloves/ eye protection/ face protection.
Response:
P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P314 Get medical advice/ attention if you feel unwell.
P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P391 Collect spillage.
Storage:
P403 + P235 Store in a well-ventilated place. Keep cool.
Disposal:

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

CAS-No. : 98-08-8

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
α,α,α -trifluorotoluene	98-08-8*	$\geq 90 - \leq 100$	-

* Indicates that the identifier is a CAS No.

Actual concentration is withheld as a trade secret

SECTION 4. FIRST AID MEASURES

General advice : 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. Consult a physician.

In case of eye contact : After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

If swallowed : After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

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 : Carbon dioxide (CO₂)
Dry powder

Sigma-Aldrich - 547948

Page 3 of 15

Unsuitable extinguishing media : Foam
Water

Specific hazards during fire fighting : Combustible.

Pay attention to flashback.

Vapours are heavier than air and may spread along floors.

Development of hazardous combustion gases or vapours possible in the event of fire.

Forms explosive mixtures with air at ambient temperatures.

Hazardous combustion products : Carbon oxides

Hydrogen fluoride

Specific extinguishing methods : No data available

Further information : Remove container from danger zone and cool with water.
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 : Advice for non-emergency personnel:
Do not breathe vapours, aerosols.

Sigma-Aldrich - 547948

Page 4 of 15

emergency procedures Avoid substance contact.
Ensure adequate ventilation.
Keep away from heat and sources of ignition.
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.
Risk of explosion.

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 GHS label elements

Advice on protection against fire and explosion : Keep away from open flames, hot surfaces and sources of ignition.
Take precautionary measures against static discharge.

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

Further information on storage conditions : Keep container tightly closed in a dry and well-ventilated place.
Keep away from heat and sources of ignition.

Storage class : 3, Flammable liquids

Recommended storage temperature : Recommended storage temperature see product label.

Packaging material : Suitable material: Poly-lined Steel Drum

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 : 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).
Safety glasses

Skin and body protection : Flame retardant antistatic protective clothing.

Hygiene measures : Change contaminated clothing. Preventive skin protection recommended. Wash hands after working

with substance.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance	: liquid (68 °F / 20 °C, 1,013 hPa)
Colour	: colourless
Odour	: No data available
Odour Threshold	: No data available
pH	: No data available
Melting point/ range	: -20 °F / -29 °C Method: lit.
Boiling point/boiling range	: 216 °F / 102 °C Method: lit.
Flash point	: 46 °F / 8 °C Method: Regulation (EC) No. 440/2008, Annex, A.9, closed cup GLP: yes
Evaporation rate	: No data available
Flammability (solid, gas)	: No data available
Flammability (liquids)	: No data available
Burning rate	: No data available
Self-ignition	: Method: DIN 51794 GLP: yes not auto-flammable
Upper explosion limit / Upper flammability limit	: No data available
Lower explosion limit / Lower flammability limit	: No data available
Vapour pressure	: 69.99 hPa (68 °F / 20 °C) Method: OECD Test Guideline 104 GLP: yes
Relative vapour density	: 5.04 (Air = 1.0)

Sigma-Aldrich - 547948

Page 7 of 15

Relative density	: No data available
Density	: 1.19 g/cm ³ (68 °F / 20 °C) Method: lit.
Solubility(ies)	
Water solubility	: 0.151 g/l (68 °F / 20 °C) Method: OECD Test Guideline 105 GLP: yes
Partition coefficient: n-octanol/water	: Pow: 1,031 (68 °F / 20 °C) log Pow: 3.01 (68 °F / 20 °C) Method: OECD Test Guideline 117 GLP: yes Bioaccumulation is not expected.
Autoignition temperature	: 1202 °F / 650 °C
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	: none
Molecular weight	: 146.11 g/mol
Particle characteristics	
Particle size	: No data available

SECTION 10. STABILITY AND REACTIVITY

Reactivity	: Vapours may form explosive mixture with air.
Chemical stability	: The product is chemically stable under standard ambient conditions (room temperature) .
Possibility of hazardous reactions	: Generates dangerous gases or fumes in contact with: Water Violent reactions possible with: Strong oxidizing agents strong reducing agents Strong bases

Sigma-Aldrich - 547948

Page 8 of 15

Conditions to avoid : Warming.

Incompatible materials : No data available

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

SECTION 11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Mouse - 10,000 mg/kg

Remarks: Behavioral:General anesthetic.

Behavioral:Excitement.

Behavioral:Muscle weakness.

LC50 Inhalation - Rat - 4 h - 70,810 mg/m³ - vapour

LD50 Dermal - Rat - > 2,000 mg/kg

(OECD Test Guideline 402)

No data available

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 4 h

(OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation - 72 h

(OECD Test Guideline 405)

Respiratory or skin sensitization

Direct Peptide Reactivity Assay (DPRA)

Result: Not a skin sensitizer.

(OECD Test Guideline 442C)

Germ cell mutagenicity

Test Type: reverse mutation assay

Test system: TA1535

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

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

May cause damage to organs through prolonged or repeated exposure.

Aspiration hazard

No data available

11.2 Additional Information

RTECS: XT9450000

Central nervous system depression, Drowsiness, Dizziness, To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity

Components:

α,α,α -trifluorotoluene:

Toxicity to fish : LC50 (*Oryzias latipes*): 19.4 mg/l
Exposure time: 96 h
Remarks: (ECHA)

Toxicity to daphnia and : EC50 (*Daphnia magna* (Water flea)): 3.11 mg/l
other aquatic : Exposure time: 48 h
invertebrates : Test Type: semi-static test
Analytical monitoring: yes
Method: OECD Test Guideline 202
GLP: yes

Toxicity to algae/aquatic : EC50 (*Pseudokirchneriella subcapitata*): 5.4 mg/l
plants : Exposure time: 72 h
Test Type: static test
Analytical monitoring: yes
Method: OECD Test Guideline 201
GLP: yes

Toxicity to : EC5 (activated sludge): 10 - 100 mg/l
microorganisms : Exposure time: 24 h
Remarks: (IUCLID)

Ecotoxicology Assessment

Chronic aquatic toxicity : Toxic to aquatic life with long lasting effects.

Persistence and degradability

Components:

α,α,α -trifluorotoluene:

Biodegradability : aerobic
Inoculum: activated sludge, non-adapted
Concentration: 2.4 mg/l
Result: Not readily biodegradable.
Biodegradation: 74 %
Exposure time: 28 d
Method: OECD Test Guideline 301D
GLP: yes

Bioaccumulative potential

Components:

α,α,α -trifluorotoluene:

Bioaccumulation : Remarks: No data available

Partition coefficient: n-octanol/water : Pow: 1,031 (68 °F / 20 °C)
log Pow: 3.01 (68 °F / 20 °C)
pH: 10
Method: OECD Test Guideline 117
GLP: yes
Remarks: Bioaccumulation is not expected.

Mobility in soil

Components:

α,α,α -trifluorotoluene:

Stability in soil : Remarks: No data available

Other adverse effects

Components:

α,α,α -trifluorotoluene:

Additional ecological information : Biological effects:

Forms toxic and corrosive mixtures with water even if diluted.

Possible decomposition products in case of hydrolysis are:

Hydrogen fluoride

Further information on ecology

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 2338
Proper shipping name : Benzotrifluoride
Class : 3
Packing group : II
Labels : Class 3 - Flammable liquids
Packing instruction (cargo : 364
aircraft)
Packing instruction : 353
(passenger aircraft)

IMDG-Code

UN number : UN 2338
Proper shipping name : BENZOTRIFLUORIDE

Class : 3
Packing group : II
Labels : 3
EmS Code : F-E, S-D
Marine pollutant : yes

Transport in bulk according to IMO instruments

Not applicable for product as supplied.

National Regulations

49 CFR

UN/ID/NA number : UN 2338
Proper shipping name : Benzotrifluoride

Class : 3

Packing group : II

Sigma-Aldrich - 547948

Page 12 of 15

Labels : Class 3 - Flammable liquids
ERG Code : 127
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 : Fire Hazard
Chronic 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

α,α,α-trifluorotoluene 98-08-8

Pennsylvania Right To Know

α,α,α-trifluorotoluene 98-08-8

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:

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.

Revision Date : 07/15/2026

US / EN