

## SAFETY DATA SHEET

Version 6.11  
Revision Date 09/08/2024  
Print Date 09/09/2024

**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name :  $\alpha,\alpha,\alpha$ -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

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**

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

**SECTION 2: Hazards identification****2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Flammable liquids (Category 2), H225  
Specific target organ toxicity - repeated exposure (Category 2), H373  
Short-term (acute) aquatic hazard (Category 2), H401

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Long-term (chronic) aquatic hazard (Category 2), H411

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 Statements

H225

Highly flammable liquid and vapor.

H373

May cause damage to organs through prolonged or repeated exposure.

H411

Toxic to aquatic life with long lasting effects.

Precautionary Statements

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 vapors.

P273

Avoid release to the environment.

P280

Wear protective gloves/ eye protection/ face protection.

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.

P403 + P235

Store in a well-ventilated place. Keep cool.

P501

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

## 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

### SECTION 3: Composition/information on ingredients

#### 3.1 Substances

Synonyms : Benzotrifluoride

Formula : C<sub>7</sub>H<sub>5</sub>F<sub>3</sub>

Molecular weight : 146.11 g/mol

CAS-No. : 98-08-8

EC-No. : 202-635-0

Index-No. : 602-056-00-7

Component	Classification	Concentration
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<b><math>\alpha,\alpha,\alpha</math>-trifluorotoluene</b>		
	Flam. Liq. 2; STOT RE 2; Aquatic Acute 2; Aquatic Chronic 2; H225, H373, H401, H411	<= 100 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

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## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

#### General advice

Show this material 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.

### 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

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## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

#### Suitable extinguishing media

Carbon dioxide (CO<sub>2</sub>) Dry powder

#### Unsuitable extinguishing media

Foam Water

### 5.2 Special hazards arising from the substance or mixture

Carbon oxides

Hydrogen fluoride

Combustible.

Pay attention to flashback.

Vapors are heavier than air and may spread along floors.

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Development of hazardous combustion gases or vapours possible in the event of fire.  
Forms explosive mixtures with air at ambient temperatures.

### **5.3 Advice for firefighters**

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

### **5.4 Further information**

Remove container from danger zone and cool with water. Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

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## **SECTION 6: Accidental release measures**

### **6.1 Personal precautions, protective equipment and emergency procedures**

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert. For personal protection see section 8.

### **6.2 Environmental precautions**

Do not let product enter drains. Risk of explosion.

### **6.3 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.

### **6.4 Reference to other sections**

For disposal see section 13.

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## **SECTION 7: Handling and storage**

### **7.1 Precautions for safe handling**

#### **Advice on safe handling**

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

#### **Advice on protection against fire and explosion**

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

#### **Hygiene measures**

Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

For precautions see section 2.2.

### **7.2 Conditions for safe storage, including any incompatibilities**

#### **Storage conditions**

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.

#### **Storage class**

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Storage class (TRGS 510): 3: Flammable liquids

### 7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

### 8.2 Exposure controls

#### Appropriate engineering controls

Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

#### Personal protective equipment

##### Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

##### Skin protection

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](http://www.kcl.de)).

Full contact

Material: Viton®

Minimum layer thickness: 0.7 mm

Break through time: 480 min

Material tested: Vitoject® (KCL 890 / Aldrich Z677698, Size M)

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](http://www.kcl.de)).

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.4 mm

Break through time: 120 min

Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

##### Body Protection

Flame retardant antistatic protective clothing.

##### Respiratory protection

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.  
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.

### **Control of environmental exposure**

Do not let product enter drains. Risk of explosion.

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## **SECTION 9: Physical and chemical properties**

### **9.1 Information on basic physical and chemical properties**

a) Appearance	Form: clear, liquid Color: colorless
b) Odor	No data available
c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/ range: -29 °C (-20 °F) - lit.
f) Initial boiling point and boiling range	102 °C 216 °F - lit.
g) Flash point	8 °C (46 °F) - closed cup - Regulation (EC) No. 440/2008, Annex, A.9
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	No data available
k) Vapor pressure	69.99 hPa at 20 °C (68 °F) - OECD Test Guideline 104
l) Vapor density	5.04 - (Air = 1.0)
m) Density	1.19 g/cm <sup>3</sup> at 20 °C (68 °F) - lit.
Relative density	No data available
n) Water solubility	0.151 g/l at 20 °C (68 °F) - OECD Test Guideline 105
o) Partition coefficient: n-octanol/water	Pow: 1,031; log Pow: 3.01 at 20 °C (68 °F) - OECD Test Guideline 117 - Bioaccumulation is not expected.
p) Autoignition temperature	not auto-flammable
q) Decomposition temperature	No data available

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- r) Viscosity No data available  
s) Explosive properties No data available  
t) Oxidizing properties none

## 9.2 Other safety information

Relative vapor density 5.04 - (Air = 1.0)

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

Vapors may form explosive mixture with air.

### 10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

### 10.3 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

### 10.4 Conditions to avoid

Warming.

### 10.5 Incompatible materials

No data available

### 10.6 Hazardous decomposition products

In the event of fire: see section 5

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## 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/m<sup>3</sup> - vapor

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 ingredient 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 ingredient 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



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## SECTION 12: Ecological information

### 12.1 Toxicity

Toxicity to fish	LC50 - <i>Oryzias latipes</i> - 19.4 mg/l - 96 h Remarks: (ECHA)
Toxicity to daphnia and other aquatic invertebrates	semi-static test EC50 - <i>Daphnia magna</i> (Water flea) - 3.11 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	static test EC50 - <i>Pseudokirchneriella subcapitata</i> - 5.4 mg/l - 72 h (OECD Test Guideline 201)
Toxicity to bacteria	EC5 - activated sludge - 10 - 100 mg/l - 24 h Remarks: (IUCLID)

### 12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 28 d Result: 74 % - Not readily biodegradable. (OECD Test Guideline 301D)
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### 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 Endocrine disrupting properties

No data available

### 12.7 Other adverse effects

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.

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## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

#### Product

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.

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## SECTION 14: Transport information

#### DOT (US)

UN number: 2338    Class: 3    Packing group: II  
Proper shipping name: Benzotrifluoride  
Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

#### IMDG

UN number: 2338    Class: 3    Packing group: II    EMS-No: F-E, S-D  
Proper shipping name: BENZOTRIFLUORIDE  
Marine pollutant : yes

#### IATA

UN number: 2338    Class: 3    Packing group: II  
Proper shipping name: Benzotrifluoride

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## 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

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**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 ingredients of this product are reported in the following inventories:**

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.

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**SECTION 16: Other information****Further information**

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](http://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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