

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Version 6.7

Revision Date 02.11.2023

Print Date 03.05.2025

GENERIC EU MSDS - NO COUNTRY SPECIFIC DATA - NO OEL DATA

## SECTION 1: Identification of the substance/mixture and of the company/undertaking

### 1.1 Product identifiers

Product name : 2-Ethynyl-*a,a,a*-trifluorotoluene

Product Number : 521183

Brand : Aldrich

REACH No. : A registration number is not available for this substance as the substance or its uses are exempted from registration, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

CAS-No. : 704-41-6

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

Identified uses : Laboratory chemicals, Manufacture of substances

### 1.3

CHEMIKART

### 1.4 Emergency telephone

Emergency Phone # : 000 800 1007 141 (CHEMTREC)

## SECTION 2: Hazards identification

### 2.1 Classification of the substance or mixture

**Classification according to Regulation (EC) No 1272/2008**

Flammable liquids (Category 3), H226

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

### 2.2 Label elements

**Labelling according Regulation (EC) No 1272/2008**

Pictogram

Signal Word	Warning
Hazard statement(s) H226	Flammable liquid and vapor.
Precautionary statement(s)	none
Supplemental Hazard Statements	none

### 2.3 Other hazards

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

Ecological information:

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

Toxicological information:

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

---

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Synonyms : 1-Ethynyl-2-trifluoromethylbenzene

Formula : C<sub>9</sub>H<sub>5</sub>F<sub>3</sub>  
Molecular weight : 170,13 g/mol  
CAS-No. : 704-41-6

No components need to be disclosed according to the applicable regulations.

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

---

## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

#### General advice

Consult a physician. Show this material safety data sheet to the doctor in attendance.

#### If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

**In case of skin contact**

Wash off with soap and plenty of water. Consult a physician.

**In case of eye contact**

Flush eyes with water as a precaution.

**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

---

**SECTION 5: Firefighting measures****5.1 Extinguishing media****Suitable extinguishing media**

Small (incipient) fires must be extinguished with alcohol resistant foam, dry chemical powder or carbon dioxide. Large amounts of water are ineffective. Cool containers with large amounts of water.

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

Carbon oxides  
Hydrogen fluoride

**5.3 Advice for firefighters**

Wear self-contained breathing apparatus for firefighting if necessary.

**5.4 Further information**

Use water spray to cool unopened containers.

---

**SECTION 6: Accidental release measures****6.1 Personal precautions, protective equipment and emergency procedures**

Avoid breathing vapors, mist or gas. Remove all sources of ignition. Beware of vapors accumulating to form explosive concentrations. Vapors can accumulate in low 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**

Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

**6.4 Reference to other sections**

For disposal see section 13.

---

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

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

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

Avoid inhalation of vapor or mist.

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

Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

#### **Hygiene measures**

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

For precautions see section 2.2.

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

#### **Storage conditions**

Store in cool place. 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.

#### **Storage class**

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

---

## **SECTION 8: Exposure controls/personal protection**

### **8.1 Control parameters**

#### **Ingredients with workplace control parameters**

### **8.2 Exposure controls**

#### **Personal protective equipment**

##### **Eye/face protection**

Face shield and safety glasses 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.

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

##### **Body Protection**

Impervious clothing, Flame retardant antistatic protective clothing., 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.

---

## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

- |   |  |
|---|--|
| a) Physical state                               | liquid   |
| b) Color  | colorless  |
| c) Odor   | No data available  |
| d) Melting point/freezing point                 | No data available  |
| e) Initial boiling point and boiling range      | 45 °C at 10 hPa - lit.   |
| f) Flammability (solid, gas)                    | No data available  |
| g) Upper/lower flammability or explosive limits | No data available  |
| h) Flash point                                  | 25 °C - closed cup   |
| i) Autoignition temperature                     | No data available  |
| j) Decomposition temperature                    | No data available  |
| k) pH   | No data available  |
| l) Viscosity                                    | Viscosity, kinematic: No data available<br>Viscosity, dynamic: No data available |
| m) Water solubility                             | No data available  |
| n) Partition coefficient: n-octanol/water       | No data available  |
| o) Vapor pressure                               | No data available  |
| p) Density                                      | 1,222 g/cm <sup>3</sup> at 25 °C - lit.  |
| Relative density                                | No data available  |
| q) Relative vapor density                       | No data available  |

r) Particle characteristics No data available

s) Explosive properties No data available

t) Oxidizing properties No data available

## **9.2 Other safety information**

No data available

---

## **SECTION 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**

Heat, flames and sparks.

### **10.5 Incompatible materials**

Strong oxidizing agents

### **10.6 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**

Remarks: No data available

#### **Serious eye damage/eye irritation**

Remarks: No data available

#### **Respiratory or skin sensitization**

No data available

#### **Germ cell mutagenicity**

No data available

#### **Carcinogenicity**

No data available

#### **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****Endocrine disrupting properties****Product:**

Assessment

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

No data available

---

**SECTION 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**

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

**12.6 Endocrine disrupting properties****Product:**

Assessment

: The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

**12.7 Other adverse effects**

No data available

---

## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

#### Product

Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

#### Contaminated packaging

Dispose of as unused product.

---

## SECTION 14: Transport information

### 14.1 UN number

ADR/RID: 1993

IMDG: 1993

IATA: 1993

### 14.2 UN proper shipping name

ADR/RID: FLAMMABLE LIQUID, N.O.S. (2-Ethynyl-a ,a ,a-trifluorotoluene) (2-Ethynyl-a ,a ,a-trifluorotoluene)

IMDG: FLAMMABLE LIQUID, N.O.S. (2-Ethynyl-a ,a ,a-trifluorotoluene) (2-Ethynyl-a ,a ,a-trifluorotoluene)

IATA: Flammable liquid, n.o.s. (2-Ethynyl-a ,a ,a-trifluorotoluene) (2-Ethynyl-a ,a ,a-trifluorotoluene)

### 14.3 Transport hazard class(es)

ADR/RID: 3

IMDG: 3

IATA: 3

### 14.4 Packaging group

ADR/RID: III

IMDG: III

IATA: III

### 14.5 Environmental hazards

ADR/RID: no

IMDG Marine pollutant: no

IATA: no

### 14.6 Special precautions for user

Tunnel restriction code : (D/E)

Further information : No data available

---

## SECTION 15: Regulatory information

### 15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.

International Chemical Weapons Convention :  
(CWC) Schedules of Toxic Chemicals and  
Precursors

Restrictions on the marketing and use of certain :  
dangerous substances and preparations



Regulation (EC) No 649/2012 of the European Parliament and the Council concerning the export and import of dangerous chemicals :  
Candidate List of Substances of Very High Concern for Authorisation :

**National legislation**

Seveso III: Directive 2012/18/EU of the European Parliament and of the Council on the control of major-accident hazards involving dangerous substances. P5c FLAMMABLE LIQUIDS

**15.2 Chemical Safety Assessment**

For this product a chemical safety assessment was not carried out

---

**SECTION 16: Other information**

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

H226 Flammable liquid and vapor.

CHEMIKART

## Full text of other abbreviations

ADN - European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways; ADR - Agreement concerning the International Carriage of Dangerous Goods by Road; AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; 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; GHS - Globally Harmonized System; GLP - Good Laboratory Practice; 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 Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; 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; n.o.s. - Not Otherwise Specified; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NZIoC - New Zealand Inventory of Chemicals; OECD - Organization 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; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RID - Regulations concerning the International Carriage of Dangerous Goods by Rail; SADT - Self-Accelerating Decomposition Temperature; 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

## Further information

Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. 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.

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact [mlsbranding@sial.com](mailto:mlsbranding@sial.com).

# CHEMIKART