

## Chemical Safety Data Sheet MSDS / SDS

## 4'-TRIFLUOROMETHYLPHENYL ACETYLENE

Revision Date:2025-02-01 Revision Number:1

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

## Product identifier

Product name : 4'-TRIFLUOROMETHYLPHENYL ACETYLENE  
CBnumber : CB1298543  
CAS : 705-31-7  
Synonyms : 1-Ethynyl-4-(trifluoromethyl)benzene,4-(Trifluoromethyl)phenylacetylene

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

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.  
Uses advised against : none

## Company Identification

Company : Chemicalbook  
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing  
Telephone : 400-158-6606

## SECTION 2: Hazards identification

## GHS Label elements, including precautionary statements

Symbol(GHS)



Signal word

Danger

## Precautionary statements

P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.

## Hazard statements

H225 Highly Flammable liquid and vapour

## SECTION 3: Composition/information on ingredients

## Substance

Product name : 4'-TRIFLUOROMETHYLPHENYL ACETYLENE  
Synonyms : 1-Ethynyl-4-(trifluoromethyl)benzene,4-(Trifluoromethyl)phenylacetylene  
CAS : 705-31-7

MF : C9H5F3  
MW : 170.13

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## SECTION 4: First aid measures

### Description of first aid measures

#### General advice

Consult a physician. Show this 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.

### 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

### Indication of any immediate medical attention and special treatment needed

No data available

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## SECTION 5: Firefighting measures

### 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.

### Special hazards arising from the substance or mixture

Carbon oxides, Hydrogen fluoride

### Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

### Further information

Use water spray to cool unopened containers.

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## SECTION 6: Accidental release measures

### Personal precautions, protective equipment and emergency procedures

Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.

For personal protection see section 8.

### **Environmental precautions**

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

### **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).

### **Reference to other sections**

For disposal see section 13.

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

### **Precautions for safe handling**

Avoid inhalation of vapour or mist.

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

For precautions see section 2.2.

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

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.

### **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**

### **control parameter**

#### **Hazard composition and occupational exposure limits**

Does not contain substances with occupational exposure limits.

### **Exposure controls**

#### **Appropriate engineering controls**

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

#### **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.

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## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

|  |                                  |
|--|----------------------------------|
| Appearance                                   | colourless liquid                |
| Odour  | No data available                |
| Odour Threshold                              | No data available                |
| pH   | No data available                |
| Melting point/freezing point                 | No data available                |
| Initial boiling point and boiling range      | 78 - 80 °C at 3 hPa - lit.       |
| Flash point                                  | 20,6 °C - closed cup             |
| Evaporation rate                             | No data available                |
| Flammability (solid, gas)                    | No data available                |
| Upper/lower flammability or explosive limits | No data available                |
| Vapour pressure                              | No data available                |
| Vapour density                               | No data available                |
| Relative density                             | 1,043 g/cm <sup>3</sup> at 25 °C |
| Water solubility                             | No data available                |
| Partition coefficient: n-octanol/water       | No data available                |
| Autoignition temperature                     | No data available                |
| Decomposition temperature                    | No data available                |
| Viscosity                                    | No data available                |
| Explosive properties                         | No data available                |
| Oxidizing properties                         | No data available                |
| $\lambda_{\text{max}}$                       | 249nm(EtOH)(lit.)                |

### Other safety information

No data available

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## SECTION 10: Stability and reactivity

### Reactivity

No data available

### Chemical stability

Stable under recommended storage conditions.

### Possibility of hazardous reactions

No data available

### Conditions to avoid

Heat, flames and sparks. Extremes of temperature and direct sunlight.

### Incompatible materials

Strong oxidizing agents Strong oxidizing agents, Strong acids, Alkali metals, Halogens

### Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Hydrogen fluoride

Other decomposition products - No data available In the event of fire: see section 5

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## SECTION 11: Toxicological information

### Information on toxicological effects

#### Acute toxicity

No data available

#### Skin corrosion/irritation

No data available

#### Serious eye damage/eye irritation

No data available

#### Respiratory or skin sensitisation

No data available

#### Germ cell mutagenicity

No data available

#### 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.

#### 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

**Additional Information**

RTECS: Not available

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

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## SECTION 12: Ecological information

**Toxicity**

No data available

**Persistence and degradability**

No data available

**Bioaccumulative potential**

No data available

**Mobility in soil**

No data available

**Results of PBT and vPvB assessment**

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

**Other adverse effects**

No data available

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## SECTION 13: Disposal considerations

**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.

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## SECTION 14: Transport information

**UN number**

ADR/RID: 1993 IMDG: 1993 IATA: 1993

### UN proper shipping name

ADR/RID: FLAMMABLE LIQUID, N.O.S. (4-Ethynyl-  $\alpha, \alpha, \alpha$ -trifluorotoluene) IMDG: FLAMMABLE LIQUID, N.O.S. (4-Ethynyl-  $\alpha, \alpha, \alpha$ -trifluorotoluene) IATA: Flammable liquid, n.o.s. (4-Ethynyl-  $\alpha, \alpha, \alpha$ -trifluorotoluene)

### Transport hazard class(es)

ADR/RID: 3 IMDG: 3 IATA: 3

### Packaging group

ADR/RID: II IMDG: II IATA: II

### Environmental hazards

ADR/RID: no IMDG Marine pollutant: no IATA: no

### Special precautions for user

No data available

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## SECTION 15: Regulatory information

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

#### Regulations on the Safety Management of Hazardous Chemicals

China Catalog of Hazardous chemicals 2015:Not Listed. website: <https://www.mem.gov.cn/>

#### Measures for Environmental Management of New Chemical Substances

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Not Listed. website: <https://www.mee.gov.cn/>

EC Inventory:Not Listed.

European Inventory of Existing Commercial Chemical Substances (EINECS):Not Listed. website: <https://echa.europa.eu/>

Korea Existing Chemicals List (KECL):Not Listed. website: <http://ncis.nier.go.kr>

New Zealand Inventory of Chemicals (NZIoC):Not Listed. website: <https://www.epa.govt.nz/>

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Not Listed. website: <https://emb.gov.ph/>

United States Toxic Substances Control Act (TSCA) Inventory:Not Listed. website: <https://www.epa.gov/>

Vietnam National Chemical Inventory:Not Listed. website: <https://chemicaldata.gov.vn/>

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## SECTION 16: Other information

### Abbreviations and acronyms

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

CAS: Chemical Abstracts Service

EC50: Effective Concentration 50%

IATA: International Air Transportation Association

IMDG: International Maritime Dangerous Goods

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

STEL: Short term exposure limit

TWA: Time Weighted Average

## References

- 【1】 CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>
- 【2】 ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>
- 【3】 ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>
- 【4】 eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:  
[http://www.echemportal.org/echemportal/index?pageID=0&request\\_locale=en](http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en)
- 【5】 ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>
- 【6】 Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>
- 【7】 HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>
- 【8】 IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>
- 【9】 IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>
- 【10】 Sigma-Aldrich, website: <https://www.sigmaaldrich.com/>

### Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.