

**SECTION 1: IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING****1.1. Product identifier**

Product Description: 2-(Trifluoromethyl)phenylacetylene  
Cat No. : H53478  
CAS No 704-41-6  
Molecular Formula C9 H5 F3

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

Recommended Use Laboratory chemicals.  
Uses advised against No Information available

**1.3. Details of the supplier of the safety data sheet****Company**

Thermo Fisher (Kandel) GmbH  
Erlenbachweg 2, 76870 Kandel, Germany  
Tel: +49 (0) 721 84007 280  
Fax: +49 (0) 721 84007 300

**Swiss distributor - Fisher Scientific AG**  
Neuhofstrasse 11, CH 4153 Reinach  
Tel: +41 (0) 56 618 41 11  
<https://www.fishersci.ch/ch/en/customer-help-support/forms/email-us.html>

E-mail address begel.sdsdesk@thermofisher.com

**1.4. Emergency telephone number**

For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11  
Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99  
**CHEMTREC** Tel. No.**US**:001-800-424-9300 / **Europe**:001-703-527-3887

customers in Switzerland:  
Tox Info Suisse Emergency Number: **145 (24hr)**  
Tox Info Suisse: +41-44 251 51 51 (Emergency number from abroad)  
Chemtrec (24h) Toll-Free: 0800 564 402  
Chemtrec Local: +41-43 508 20 11 (Zurich)

**SECTION 2: HAZARDS IDENTIFICATION****2.1. Classification of the substance or mixture**

CLP Classification - Regulation (EC) No 1272/2008

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## Physical hazards

Flammable liquids

Category 3 (H226)

## Health hazards

Based on available data, the classification criteria are not met

## Environmental hazards

Based on available data, the classification criteria are not met

*Full text of Hazard Statements: see section 16*

## 2.2. Label elements



Signal Word

Warning

## Hazard Statements

H226 - Flammable liquid and vapor

## Precautionary Statements

P403 + P233 - Store in a well-ventilated place. Keep container tightly closed  
P303 + P361 + P353 - IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower  
P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking

## 2.3. Other hazards

This product does not contain any known or suspected endocrine disruptors

## **SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS**

### 3.1. Substances

Component	CAS No	EC No	Weight %	CLP Classification - Regulation (EC) No 1272/2008
2-Ethynyl-.alpha.,.alpha.,.alpha.-trifluorotoluene	704-41-6		<=100	Flam. Liq. 3 (H226)

*Full text of Hazard Statements: see section 16*

## **SECTION 4: FIRST AID MEASURES**

### 4.1. Description of first aid measures

General Advice

If symptoms persist, call a physician.

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<b>Eye Contact</b>	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.
<b>Skin Contact</b>	Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, call a physician.
<b>Ingestion</b>	Clean mouth with water and drink afterwards plenty of water.
<b>Inhalation</b>	Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur.
<b>Self-Protection of the First Aider</b>	Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.

## **4.2. Most important symptoms and effects, both acute and delayed**

Difficulty in breathing. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

## **4.3. Indication of any immediate medical attention and special treatment needed**

**Notes to Physician** Treat symptomatically.

## **SECTION 5: FIREFIGHTING MEASURES**

### **5.1. Extinguishing media**

#### **Suitable Extinguishing Media**

Water mist may be used to cool closed containers.

#### **Extinguishing media which must not be used for safety reasons**

No information available.

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

Flammable. Containers may explode when heated. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back.

#### **Hazardous Combustion Products**

None under normal use conditions.

### **5.3. Advice for firefighters**

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

## **SECTION 6: ACCIDENTAL RELEASE MEASURES**

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

Ensure adequate ventilation. Use personal protective equipment as required. Remove all sources of ignition. Take precautionary measures against static discharges.

### **6.2. Environmental precautions**

Should not be released into the environment. See Section 12 for additional Ecological Information.

### **6.3. Methods and material for containment and cleaning up**

Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. Remove all sources of ignition. Use

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spark-proof tools and explosion-proof equipment.

## 6.4. Reference to other sections

Refer to protective measures listed in Sections 8 and 13.

## **SECTION 7: HANDLING AND STORAGE**

### 7.1. Precautions for safe handling

Wear personal protective equipment/face protection. Ensure adequate ventilation. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation. Keep away from open flames, hot surfaces and sources of ignition. Use only non-sparking tools. Take precautionary measures against static discharges.

#### **Hygiene Measures**

Handle in accordance with good industrial hygiene and safety practice. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Wash hands before breaks and after work.

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

Store under an inert atmosphere. Keep container tightly closed in a dry and well-ventilated place. Keep away from heat, sparks and flame.

**Technical Rules for Hazardous Substances (TRGS) 510** Class 3  
**Storage Class (LGK) (Germany)**

**Switzerland - Storage of hazardous substances** Storage class - SC 3  
<https://www.kvu.ch/de/themen/stoffe-und-produkte>  
<https://www.kvu.ch/fr/themes/substances-et-produits>  
<https://www.kvu.ch/it/temi/sostanze-e-prodotti>

### 7.3. Specific end use(s)

Use in laboratories

## **SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION**

### 8.1. Control parameters

#### **Exposure limits**

This product, as supplied, does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies

#### **Biological limit values**

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific regulatory bodies

#### **Monitoring methods**

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents.

MDHS70 General methods for sampling airborne gases and vapours

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MDHS 88 Volatile organic compounds in air. Laboratory method using diffusive samplers, solvent desorption and gas chromatography

MDHS 96 Volatile organic compounds in air - Laboratory method using pumped solid sorbent tubes, solvent desorption and gas chromatography

## Derived No Effect Level (DNEL) / Derived Minimum Effect Level (DMEL)

No information available

## Predicted No Effect Concentration (PNEC)

No information available.

## 8.2. Exposure controls

### Engineering Measures

Ensure adequate ventilation, especially in confined areas. Use explosion-proof electrical/ventilating/lighting/equipment. Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source

### Personal protective equipment

#### Eye Protection

Wear safety glasses with side shields (or goggles) (European standard - EN 166)

#### Hand Protection

Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments (minimum requirement)
Nitrile rubber	See manufacturers recommendations	-	EN 374	
Neoprene				
Natural rubber				
PVC				

#### Skin and body protection

Long sleeved clothing.

Inspect gloves before use. observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information) gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion. gloves with care avoiding skin contamination.

#### Respiratory Protection

When workers are facing concentrations above the exposure limit they must use appropriate certified respirators.  
To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

#### Large scale/emergency use

Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced  
**Recommended Filter type:** Organic gases and vapours filter Type A Brown conforming to EN14387

#### Small scale/Laboratory use

Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.  
**Recommended half mask:-** Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 141  
When RPE is used a face piece Fit Test should be conducted

#### Environmental exposure controls

No information available.

## SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

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## 9.1. Information on basic physical and chemical properties

Physical State	Liquid	
Appearance	Colorless	
Odor	No information available	
Odor Threshold	No data available	
Melting Point/Range	No data available	
Softening Point	No data available	
Boiling Point/Range	45 °C / 113 °F	
Flammability (liquid)	Flammable	
Flammability (solid,gas)	Not applicable	
Explosion Limits	No data available	
Flash Point	25 °C / 77 °F	
Autoignition Temperature	No data available	
Decomposition Temperature	No data available	
pH	No information available	
Viscosity	No data available	
Water Solubility	No information available	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)	No data available	
Vapor Pressure	1.222 g/cm3	
Density / Specific Gravity	@ 20 °C	
Bulk Density	Liquid	
Vapor Density	(Air = 1.0)	
Particle characteristics	Not applicable (liquid)	

## 9.2. Other information

Molecular Formula	C9 H5 F3
Molecular Weight	170.13
Explosive Properties	explosive air/vapour mixtures possible

## SECTION 10: STABILITY AND REACTIVITY

### 10.1. Reactivity

None known, based on information available

### 10.2. Chemical stability

Air sensitive.

### 10.3. Possibility of hazardous reactions

Hazardous Polymerization	No information available.
Hazardous Reactions	None under normal processing.

### 10.4. Conditions to avoid

Keep away from open flames, hot surfaces and sources of ignition.

### 10.5. Incompatible materials

None known.

### 10.6. Hazardous decomposition products

None under normal use conditions.

## SECTION 11: TOXICOLOGICAL INFORMATION

### 11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

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## Product Information

### (a) acute toxicity;

Oral	No data available
Dermal	No data available
Inhalation	No data available

(b) skin corrosion/irritation; No data available

(c) serious eye damage/irritation; No data available

### (d) respiratory or skin sensitization;

Respiratory	No data available
Skin	No data available

(e) germ cell mutagenicity; No data available

(f) carcinogenicity; No data available

There are no known carcinogenic chemicals in this product

(g) reproductive toxicity; No data available

(h) STOT-single exposure; No data available

(i) STOT-repeated exposure; No data available

Target Organs No information available.

(j) aspiration hazard; No data available

**Symptoms / effects, both acute and delayed** Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting.

## 11.2. Information on other hazards

### Endocrine Disrupting Properties

Assess endocrine disrupting properties for human health. This product does not contain any known or suspected endocrine disruptors.

## **SECTION 12: ECOLOGICAL INFORMATION**

### 12.1. Toxicity

#### Ecotoxicity effects

Contains no substances known to be hazardous to the environment or that are not degradable in waste water treatment plants.

### 12.2. Persistence and degradability

Persistence No information available

Persistence Persistence is unlikely, based on information available.

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<b>12.3. Bioaccumulative potential</b>	Bioaccumulation is unlikely
<b>12.4. Mobility in soil</b>	The product contains volatile organic compounds (VOC) which will evaporate easily from all surfaces. Will likely be mobile in the environment due to its volatility. Disperses rapidly in air
<b>12.5. Results of PBT and vPvB assessment</b>	No data available for assessment.
<b>12.6. Endocrine disrupting properties</b>	
<b>Endocrine Disruptor Information</b>	This product does not contain any known or suspected endocrine disruptors
<b>12.7. Other adverse effects</b>	
<b>Persistent Organic Pollutant</b>	This product does not contain any known or suspected substance
<b>Ozone Depletion Potential</b>	This product does not contain any known or suspected substance

## SECTION 13: DISPOSAL CONSIDERATIONS

### 13.1. Waste treatment methods

<b>Waste from Residues/Unused Products</b>	Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.
<b>Contaminated Packaging</b>	Dispose of this container to hazardous or special waste collection point. Empty containers retain product residue, (liquid and/or vapor), and can be dangerous. Keep product and empty container away from heat and sources of ignition.
<b>European Waste Catalogue (EWC)</b>	According to the European Waste Catalog, Waste Codes are not product specific, but application specific.
<b>Other Information</b>	Waste codes should be assigned by the user based on the application for which the product was used. Do not flush to sewer. Can be landfilled or incinerated, when in compliance with local regulations.
<b>Switzerland - Waste Ordinance</b>	Disposal should be in accordance with applicable regional, national and local laws and regulations. Ordinance on the Avoidance and the Disposal of Waste (Waste Ordinance, ADWO) SR 814.600 <a href="https://www.fedlex.admin.ch/eli/cc/2015/891/en">https://www.fedlex.admin.ch/eli/cc/2015/891/en</a>

## SECTION 14: TRANSPORT INFORMATION

### IMDG/IMO

<b>14.1. UN number</b>	UN1993
<b>14.2. UN proper shipping name</b>	Flammable liquid, n.o.s. (2-(Trifluoromethyl)phenylacetylene)
<b>Technical Shipping Name</b>	
<b>14.3. Transport hazard class(es)</b>	3
<b>14.4. Packing group</b>	III

### ADR

<b>14.1. UN number</b>	UN1993
<b>14.2. UN proper shipping name</b>	Flammable liquid, n.o.s. (2-(Trifluoromethyl)phenylacetylene)
<b>Technical Shipping Name</b>	
<b>14.3. Transport hazard class(es)</b>	3
<b>14.4. Packing group</b>	III

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## IATA

<b>14.1. UN number</b>	UN1993
<b>14.2. UN proper shipping name</b>	Flammable liquid, n.o.s. (2-(Trifluoromethyl)phenylacetylene)
<b>14.3. Transport hazard class(es)</b>	3
<b>14.4. Packing group</b>	III
<b>14.5. Environmental hazards</b>	No hazards identified
<b>14.6. Special precautions for user</b>	No special precautions required.
<b>14.7. Maritime transport in bulk according to IMO instruments</b>	Not applicable, packaged goods

## SECTION 15: REGULATORY INFORMATION

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

#### International Inventories

Europe (EINECS/ELINCS/NLP), China (IECSC), Taiwan (TCSI), Korea (KECL), Japan (ENCS), Japan (ISHL), Canada (DSL/NDSL), Australia (AICS), New Zealand (NZIoC), Philippines (PICCS). US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

Component	CAS No	EINECS	ELINCS	NLP	IECSC	TCSI	KECL	ENCS	ISHL
2-Ethynyl-.alpha. ,.alpha. ,.alpha.-trifluorotoluene	704-41-6	-	-	-	-	X	-	-	-

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
2-Ethynyl-.alpha. ,.alpha. ,.alpha.-trifluorotoluene	704-41-6	-	-	-	-	-	-	-

Legend: X - Listed '-' - Not Listed

KECL - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

#### Authorisation/Restrictions according to EU REACH

Not applicable

Component	CAS No	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization	REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
2-Ethynyl-.alpha. ,.alpha. ,.alpha.-trifluorotoluene	704-41-6	-	-	-

#### Seveso III Directive (2012/18/EC)

Component	CAS No	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements
2-Ethynyl-.alpha. ,.alpha. ,.alpha.-trifluorotoluene	704-41-6	Not applicable	Not applicable

#### Regulation (EC) No 649/2012 of the European Parliament and of the Council of 4 July 2012 concerning the export and import of dangerous chemicals

Not applicable

Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?

See table for values

Component	OECD PFAS	US (EPA) PFAS	EU (ECHA) PFAS	UK (HSE) PFAS	Chemsec PFAS (Sin)

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					List)
2-Ethynyl-.alpha. ,.alpha. ,.alpha.-trifluorotoluene (CAS #: 704-41-6)	-	-	Listed	Listed	-

## PFAS Legend

Listed = Meets the PFAS definition of the named authority

Take note of Directive 98/24/EC on the protection of the health and safety of workers from the risks related to chemical agents at work .

## National Regulations

**UK** - Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment

**WGK Classification** Water endangering class = 3 (self classification)

## Swiss Regulations

Article 4 para. 4 of the Ordinance on the protection of young people in the workplace (SR 822.115) and Article 1 lit. f of the EAER regulation on hazardous work and young people (SR 822.115.2).

Take note on Article 13 Maternity Ordinance (SR 822.111.52) with regards expectant and nursing mothers.

## 15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

## SECTION 16: OTHER INFORMATION

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

H226 - Flammable liquid and vapor

#### Legend

**CAS** - Chemical Abstracts Service

**TSCA** - United States Toxic Substances Control Act Section 8(b) Inventory

**EINECS/ELINCS** - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

**DSL/NDSL** - Canadian Domestic Substances List/Non-Domestic Substances List

**PICCS** - Philippines Inventory of Chemicals and Chemical Substances

**ENCS** - Japanese Existing and New Chemical Substances

**IECSC** - Chinese Inventory of Existing Chemical Substances

**AICS** - Australian Inventory of Chemical Substances

**KECL** - Korean Existing and Evaluated Chemical Substances

**NZIoC** - New Zealand Inventory of Chemicals

**WEL** - Workplace Exposure Limit

**TWA** - Time Weighted Average

**ACGIH** - American Conference of Governmental Industrial Hygienists

**IARC** - International Agency for Research on Cancer

**DNEL** - Derived No Effect Level

Predicted No Effect Concentration (PNEC)

**RPE** - Respiratory Protective Equipment

**LD50** - Lethal Dose 50%

**LC50** - Lethal Concentration 50%

**EC50** - Effective Concentration 50%

**NOEC** - No Observed Effect Concentration

**POW** - Partition coefficient Octanol:Water

**PBT** - Persistent, Bioaccumulative, Toxic

**vPvB** - very Persistent, very Bioaccumulative

**ADR** - European Agreement Concerning the International Carriage of Dangerous Goods by Road

**ICAO/IATA** - International Civil Aviation Organization/International Air Transport Association

**IMO/IMDG** - International Maritime Organization/International Maritime Dangerous Goods Code

**MARPOL** - International Convention for the Prevention of Pollution from Ships

**OECD** - Organisation for Economic Co-operation and Development

**ATE** - Acute Toxicity Estimate

**BCF** - Bioconcentration factor

**VOC** - (volatile organic compound)

### **Key literature references and sources for data**

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

### **Training Advice**

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Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

Prepared By Health, Safety and Environmental Department

Revision Date 07-Mar-2024

Revision Summary New emergency telephone response service provider.

**This safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.  
COMMISSION REGULATION (EU) 2020/878 amending Annex II to Regulation (EC) No  
1907/2006 .**

**For Switzerland - Compiled in accordance with the technical provisions referred to in Annex 2,  
Number 3, ChemO (SR 813.11 - Ordinance on Protection against Dangerous Substances and  
Preparations).**

## Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

**End of Safety Data Sheet**