

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

Product Description: 4-(Trifluoromethyl)phenylacetylene
Cat No. : 435370000; 435370050
CAS No 705-31-7
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**

UK entity/business name
Fisher Scientific UK
Bishop Meadow Road,
Loughborough, Leicestershire LE11 5RG, United Kingdom

EU entity/business name
Thermo Fisher Scientific
Janssen Pharmaceuticalaan 3a, 2440 Geel, Belgium

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

SECTION 2: HAZARDS IDENTIFICATION**2.1. Classification of the substance or mixture****CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567****Physical hazards**

Flammable liquids Category 2 (H225)

Health hazards

Based on available data, the classification criteria are not met

Environmental hazards

SAFETY DATA SHEET

4-(Trifluoromethyl)phenylacetylene

Revision Date 13-Oct-2023

Based on available data, the classification criteria are not met

Full text of Hazard Statements: see section 16

2.2. Label elements



Signal Word

Danger

Hazard Statements

H225 - Highly 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

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.

Eye Contact

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.

Skin Contact

Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, call a physician.

Ingestion

Clean mouth with water and drink afterwards plenty of water.

SAFETY DATA SHEET

4-(Trifluoromethyl)phenylacetylene

Revision Date 13-Oct-2023

Inhalation	Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur.
Self-Protection of the First Aider	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. Inhalation of high vapor concentrations may cause symptoms like 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

Carbon dioxide (CO₂). Powder. 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. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back. Containers may explode when heated. Vapors may form explosive mixtures with air.

Hazardous Combustion Products

Carbon monoxide (CO), Carbon dioxide (CO₂), Fluorine, Hydrogen fluoride.

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

Use personal protective equipment as required. Ensure adequate ventilation. 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 spark-proof tools and explosion-proof equipment.

6.4. Reference to other sections

Refer to protective measures listed in Sections 8 and 13.

SAFETY DATA SHEET

4-(Trifluoromethyl)phenylacetylene

Revision Date 13-Oct-2023

SECTION 7: HANDLING AND STORAGE

7.1. Precautions for safe handling

Ensure adequate ventilation. Wear personal protective equipment/face protection. Avoid ingestion and inhalation. Do not get in eyes, on skin, or on clothing. Keep away from open flames, hot surfaces and sources of ignition. Use only non-sparking tools. To avoid ignition of vapors by static electricity discharge, all metal parts of the equipment must be grounded. 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

Keep container tightly closed in a dry and well-ventilated place. Keep refrigerated. Flammables area. Keep away from heat, sparks and flame.

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

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

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

SAFETY DATA SHEET

4-(Trifluoromethyl)phenylacetylene

Revision Date 13-Oct-2023

Ensure that eyewash stations and safety showers are close to the workstation location. 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.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves.
(Refer to manufacturer/supplier for information)

Ensure 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.

Remove gloves with care avoiding skin contamination.

Respiratory Protection

No protective equipment is needed under normal use conditions.

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

Small scale/Laboratory use

Maintain adequate ventilation

Environmental exposure controls

No information available.

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

9.1. Information on basic physical and chemical properties

Physical State

Liquid

Appearance

Clear, Light yellow

Odor

No information available

Odor Threshold

No data available

Melting Point/Range

No data available

Softening Point

No data available

Boiling Point/Range

58 - 60 °C / 136.4 - 140 °F

@30Torr

Flammability (liquid)

Highly flammable

On basis of test data

Flammability (solid,gas)

Not applicable

Liquid

Explosion Limits

No data available

Flash Point

21 °C / 69.8 °F

Method - No information available

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

SAFETY DATA SHEET

4-(Trifluoromethyl)phenylacetylene

Revision Date 13-Oct-2023

Partition Coefficient (n-octanol/water)	
Vapor Pressure	No data available
Density / Specific Gravity	No data available
Bulk Density	Not applicable
Vapor Density	No data available
Particle characteristics	Liquid (Air = 1.0) Not applicable (liquid)

9.2. Other information

Molecular Formula	C9 H5 F3
Molecular Weight	170.13
Explosive Properties	Vapors may form explosive mixtures with air

SECTION 10: STABILITY AND REACTIVITY

10.1. Reactivity

None known, based on information available

10.2. Chemical stability

Stable under recommended storage conditions.

10.3. Possibility of hazardous reactions

Hazardous Polymerization	Hazardous polymerization does not occur.
Hazardous Reactions	None under normal processing.

10.4. Conditions to avoid

Incompatible products. Excess heat. Keep away from open flames, hot surfaces and sources of ignition.

10.5. Incompatible materials

Strong oxidizing agents. Strong acids.

10.6. Hazardous decomposition products

Carbon monoxide (CO). Carbon dioxide (CO₂). Fluorine. Hydrogen fluoride.

SECTION 11: TOXICOLOGICAL INFORMATION

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

Product Information	No acute toxicity information is available for this product
---------------------	---

(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
-------------	-------------------

SAFETY DATA SHEET

4-(Trifluoromethyl)phenylacetylene

Revision Date 13-Oct-2023

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	Inhalation of high vapor concentrations may cause symptoms like 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	Persistence is unlikely, based on information available.
--------------------	--

12.3. Bioaccumulative potential

Bioaccumulation is unlikely

12.4. Mobility in soil

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

12.5. Results of PBT and vPvB assessment

No data available for assessment.

12.6. Endocrine disrupting properties

Endocrine Disruptor Information	This product does not contain any known or suspected endocrine disruptors
--	---

SAFETY DATA SHEET

4-(Trifluoromethyl)phenylacetylene

Revision Date 13-Oct-2023

12.7. Other adverse effects

Persistent Organic Pollutant
Ozone Depletion Potential

This product does not contain any known or suspected substance
This product does not contain any known or suspected substance

SECTION 13: DISPOSAL CONSIDERATIONS

13.1. Waste treatment methods

Waste from Residues/Unused Products	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.
Contaminated Packaging	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.
European Waste Catalogue (EWC)	According to the European Waste Catalog, Waste Codes are not product specific, but application specific.
Other Information	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.

SECTION 14: TRANSPORT INFORMATION

IMDG/IMO

14.1. UN number	UN1993
14.2. UN proper shipping name	Flammable liquid, n.o.s.
Technical Shipping Name	4-(Trifluoromethyl)phenylacetylene
14.3. Transport hazard class(es)	3
14.4. Packing group	II

ADR

14.1. UN number	UN1993
14.2. UN proper shipping name	Flammable liquid, n.o.s.
Technical Shipping Name	4-(Trifluoromethyl)phenylacetylene
14.3. Transport hazard class(es)	3
14.4. Packing group	II

IATA

14.1. UN number	UN1993
14.2. UN proper shipping name	Flammable liquid, n.o.s.
Technical Shipping Name	4-(Trifluoromethyl)phenylacetylene
14.3. Transport hazard class(es)	3
14.4. Packing group	II

14.5. Environmental hazards

No hazards identified

14.6. Special precautions for user

No special precautions required.

14.7. Maritime transport in bulk

Not applicable, packaged goods

SAFETY DATA SHEET

4-(Trifluoromethyl)phenylacetylene

Revision Date 13-Oct-2023

according to IMO instruments

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)

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

Seveso III Directive (2012/18/EC)

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

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)

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

H225 - Highly flammable liquid and vapor

SAFETY DATA SHEET

4-(Trifluoromethyl)phenylacetylene

Revision Date 13-Oct-2023

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 Predicted No Effect Concentration (PNEC)

DNEL - Derived No Effect Level

LD50 - Lethal Dose 50%

RPE - Respiratory Protective Equipment

EC50 - Effective Concentration 50%

LC50 - Lethal Concentration 50%

POW - Partition coefficient Octanol:Water

NOEC - No Observed Effect Concentration

vPvB - very Persistent, very Bioaccumulative

PBT - Persistent, Bioaccumulative, Toxic

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

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.

Creation Date 12-Oct-2010

Revision Date 13-Oct-2023

Revision Summary Not applicable.

This safety data sheet complies with Regulation UK SI 2019/758 and UK SI 2020/1577 as amended.

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