

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

### 1.1. Product identifier

**Product name:** 4-(TRIFLUOROMETHOXY)PHENYLACETYLENE  
**CAS number:** 160542-02-9  
**Product code:** PC5952  
**Synonyms:** 1-ETHYNYL-4-(TRIFLUOROMETHOXY)BENZENE  
4-ETHYNYL-ALPHA,ALPHA,ALPHA-TRIFLUOROANISOLE

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

### 1.3. Details of the supplier of the safety data sheet

**Company name:** Apollo Scientific Ltd  
Units 3 & 4  
Parkway  
Denton  
Manchester  
M34 3SG  
UK  
**Tel:** 0161 337 9971  
**Fax:** 0161 336 6932  
**Email:** david.tideswell@apolloscientific.co.uk

### 1.4. Emergency telephone number

## Section 2: Hazards identification

### 2.1. Classification of the substance or mixture

**Classification under CLP:** Acute Tox. 4: H302; Aquatic Chronic 2: H411; Eye Irrit. 2: H319; Flam. Liq. 3: H226; Skin Sens. 1: H317

**Classification under CHIP:** -: R10; Xn: R22; Xi: R36; Sens.: R43; N: R51/53

**Most important adverse effects:** Flammable liquid and vapour. Harmful if swallowed. May cause an allergic skin reaction. Causes serious eye irritation. Toxic to aquatic life with long lasting effects.

### 2.2. Label elements

**Label elements:**

**Hazard statements:** H226: Flammable liquid and vapour.  
H302: Harmful if swallowed.  
H317: May cause an allergic skin reaction.

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H319: Causes serious eye irritation.

H411: Toxic to aquatic life with long lasting effects.

**Signal words:** Warning

**Hazard pictograms:** GHS02: Flame

GHS07: Exclamation mark

GHS09: Environmental



**Precautionary statements:** P210: Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

P273: Avoid release to the environment.

P260: Do not breathe vapours.

P280: Wear protective gloves/protective clothing/eye protection/face protection.

## 2.3. Other hazards

**Other hazards:** In use, may form flammable / explosive vapour-air mixture.

**PBT:** This product is not identified as a PBT/vPvB substance.

## Section 3: Composition/information on ingredients

### 3.1. Substances

**Chemical identity:** 4-(TRIFLUOROMETHOXY)PHENYLACETYLENE

**CAS number:** 160542-02-9

## Section 4: First aid measures

### 4.1. Description of first aid measures

**Skin contact:** Remove all contaminated clothes and footwear immediately unless stuck to skin.

Drench the affected skin with running water for 10 minutes or longer if substance is still on skin. Consult a doctor.

**Eye contact:** Bathe the eye with running water for 15 minutes. Consult a doctor.

**Ingestion:** Wash out mouth with water. Do not induce vomiting. If conscious, give half a litre of water to drink immediately. Consult a doctor.

**Inhalation:** Remove casualty from exposure ensuring one's own safety whilst doing so. Consult a doctor.

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

**Skin contact:** There may be irritation and redness at the site of contact.

**Eye contact:** There may be irritation and redness. The eyes may water profusely.

**Ingestion:** There may be soreness and redness of the mouth and throat. Nausea and stomach pain may occur. There may be vomiting.

**Inhalation:** There may be irritation of the throat with a feeling of tightness in the chest.

[cont...]

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

## Section 5: Fire-fighting measures

### 5.1. Extinguishing media

**Extinguishing media:** Carbon dioxide, dry chemical powder, foam. Suitable extinguishing media for the surrounding fire should be used. Use water spray to cool containers.

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

**Exposure hazards:** Flammable. Forms explosive air-vapour mixture. In combustion emits toxic fumes of carbon dioxide / carbon monoxide. Hydrogen fluoride (HF).

### 5.3. Advice for fire-fighters

**Advice for fire-fighters:** Wear self-contained breathing apparatus. Wear protective clothing to prevent contact with skin and eyes.

## Section 6: Accidental release measures

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

**Personal precautions:** Refer to section 8 of SDS for personal protection details. If outside do not approach from downwind. If outside keep bystanders upwind and away from danger point. Mark out the contaminated area with signs and prevent access to unauthorised personnel. Turn leaking containers leak-side up to prevent the escape of liquid. Eliminate all sources of ignition.

### 6.2. Environmental precautions

**Environmental precautions:** Do not discharge into drains or rivers. Contain the spillage using bunding.

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

**Clean-up procedures:** Absorb into dry earth or sand. Transfer to a closable, labelled salvage container for disposal by an appropriate method. Do not use equipment in clean-up procedure which may produce sparks.

### 6.4. Reference to other sections

## Section 7: Handling and storage

### 7.1. Precautions for safe handling

**Handling requirements:** Avoid direct contact with the substance. Ensure there is sufficient ventilation of the area. Do not handle in a confined space. Avoid the formation or spread of mists in the air. Smoking is forbidden. Use non-sparking tools. Only use in fume hood.

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

**Storage conditions:** Store in a cool, well ventilated area. Keep container tightly closed. Keep away from sources of ignition. Prevent the build up of electrostatic charge in the immediate area.

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Ensure lighting and electrical equipment are not a source of ignition. Light Sensitive.

Store under Argon. Recommended storage temp 2-8 °C.

**Suitable packaging:** Must only be kept in original packaging.

## 7.3. Specific end use(s)

## Section 8: Exposure controls/personal protection

### 8.1. Control parameters

**Workplace exposure limits:** No data available.

### DNEL/PNEC Values

**DNEL / PNEC** No data available.

### 8.2. Exposure controls

**Engineering measures:** Ensure there is sufficient ventilation of the area. Ensure lighting and electrical equipment are not a source of ignition.

**Respiratory protection:** Self-contained breathing apparatus must be available in case of emergency.

**Hand protection:** Impermeable gloves.

**Eye protection:** Safety glasses. Ensure eye bath is to hand.

**Skin protection:** Impermeable protective clothing.

## Section 9: Physical and chemical properties

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

**State:** Liquid

**Colour:** Colourless

**Flash point °C:** 40

**Part.coeff. n-octanol/water:** log Pow: 3.879

**Relative density:** 1.215

### 9.2. Other information

**Other information:** Refractive index: 1.4554

## Section 10: Stability and reactivity

### 10.1. Reactivity

**Reactivity:** Stable under recommended transport or storage conditions.

### 10.2. Chemical stability

**Chemical stability:** Stable under normal conditions. Stable at room temperature.

### 10.3. Possibility of hazardous reactions

**Hazardous reactions:** Hazardous reactions will not occur under normal transport or storage conditions.

### 10.4. Conditions to avoid

**Conditions to avoid:** Heat. Hot surfaces. Sources of ignition. Flames. Light.

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## 10.5. Incompatible materials

**Materials to avoid:** Strong oxidising agents. Strong acids.

## 10.6. Hazardous decomposition products

**Haz. decomp. products:** In combustion emits toxic fumes of carbon dioxide / carbon monoxide. Hydrogen fluoride (HF).

## Section 11: Toxicological information

### 11.1. Information on toxicological effects

#### Relevant hazards for substance:

Hazard	Route	Basis
Acute toxicity (ac. tox. 4)	ING	Based on test data
Serious eye damage/irritation	OPT	Based on test data
Respiratory/skin sensitisation	DRM	Based on test data

### Symptoms / routes of exposure

**Skin contact:** There may be irritation and redness at the site of contact.

**Eye contact:** There may be irritation and redness. The eyes may water profusely.

**Ingestion:** There may be soreness and redness of the mouth and throat. Nausea and stomach pain may occur. There may be vomiting.

**Inhalation:** There may be irritation of the throat with a feeling of tightness in the chest.

## Section 12: Ecological information

### 12.1. Toxicity

**Ecotoxicity values:** No data available.

### 12.2. Persistence and degradability

**Persistence and degradability:** No data available.

### 12.3. Bioaccumulative potential

**Bioaccumulative potential:** No data available.

### 12.4. Mobility in soil

**Mobility:** No data available.

### 12.5. Results of PBT and vPvB assessment

**PBT identification:** This product is not identified as a PBT/vPvB substance.

### 12.6. Other adverse effects

**Other adverse effects:** No data available.

[cont...]

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## Section 13: Disposal considerations

### 13.1. Waste treatment methods

**Disposal operations:** Transfer to a suitable container and arrange for collection by specialised disposal company. MATERIAL SHOULD BE DISPOSED OF IN ACCORDANCE WITH LOCAL, STATE AND FEDERAL REGULATIONS

**Disposal of packaging:** Dispose of as special waste in compliance with local and national regulations Observe all federal, state and local environmental regulations.

**NB:** The user's attention is drawn to the possible existence of regional or national regulations regarding disposal.

## Section 14: Transport information

### 14.1. UN number

**UN number:** \* UN1993

### 14.2. UN proper shipping name

**Shipping name:** FLAMMABLE LIQUID, N.O.S.  
(4-(Trifluoromethoxy)phenylacetylene)

### 14.3. Transport hazard class(es)

**Transport class:** \* 3

### 14.4. Packing group

**Packing group:** \* III

### 14.5. Environmental hazards

**Environmentally hazardous:** Yes

**Marine pollutant:** No

### 14.6. Special precautions for user

**Tunnel code:** D/E

**Transport category:** 3

## Section 15: Regulatory information

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

### 15.2. Chemical Safety Assessment

**Chemical safety assessment:** A chemical safety assessment has not been carried out for the substance or the mixture by the supplier.

## Section 16: Other information

### Other information

**Other information:** This safety data sheet is prepared in accordance with Commission Regulation (EU) No 453/2010.

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\* Data predicted using computational software. Toxtree - Toxic Hazard Estimation by decision tree approach. <http://ecb.jrc.ec.europa.eu/qsar/qsar-tools/index.php?c=TOXTREE>

**Phrases used in s.2 and s.3:** H226: Flammable liquid and vapour.  
H302: Harmful if swallowed.  
H317: May cause an allergic skin reaction.  
H319: Causes serious eye irritation.  
H411: Toxic to aquatic life with long lasting effects.  
R10: Flammable.  
R22: Harmful if swallowed.  
R36: Irritating to eyes.  
R43: May cause sensitisation by skin contact.  
R51/53: Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

**Legend to abbreviations:** PNEC = predicted no effect level  
DNEL = derived no effect level  
LD50 = median lethal dose  
LC50 = median lethal concentration  
EC50 = median effective concentration  
IC50 = median inhibitory concentration  
dw = dry weight  
bw = body weight  
cc = closed cup  
oc = open cup  
MUS = mouse  
GPG = guinea pig  
RBT = rabbit  
HAM = hamster  
HMN = human  
MAM = mammal  
PGN = pigeon  
IVN = intravenous  
SCU = subcutaneous  
SKN = skin  
DRM = dermal  
OCC = ocular/corneal  
PCP = physico-chemical properties

**Legal disclaimer:** The material is intended for research purposes only and should be handled exclusively by those who have been fully trained in safety, laboratory and chemical handling

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procedures. The above information is believed to be correct to the best of our knowledge. The above information is believed to be correct to the best of our knowledge at the date of its publication, but should not be considered to be all inclusive. It should be used only as a guide for safe handling, storage, transportation and disposal. We cannot guarantee that the hazards detailed in this document are the only hazards that exist for this product. This is not a warranty and Apollo Scientific Ltd shall not be held liable for any damage resulting from handling or from contact with the above product.