

**SAFETY DATA SHEET**  
4,4,4-TRIFLUOROBUTANENITRILE

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**Compilation date:** 28/05/2004  
**Revision date:** 29/10/2014  
**Revision No:** 2

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

**1.1. Product identifier**

**Product name:** 4,4,4-TRIFLUOROBUTANENITRILE  
**CAS number:** 690-95-9  
**Product code:** PC1301  
**Synonyms:** 3,3,3-TRIFLUOROPROP-1-YL CYANIDE  
4,4,4-TRIFLUOROBUTYRONITRILE

**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 CHIP:** -: R10; T: R23/24/25; Xi: R36/37/38

**Classification under CLP:** Flam. Liq. 3: H226; Acute Tox. 3: H301+311+331; STOT SE 3: H335; Eye Irrit. 2: H319;  
Skin Irrit. 2: H315

**Most important adverse effects:** Flammable. Toxic by inhalation, in contact with skin and if swallowed. Irritating to eyes, respiratory system and skin.

**2.2. Label elements**

**Label elements under CLP:**

**Hazard statements:** H226: Flammable liquid and vapour.  
H301+311+331: Toxic if swallowed, in contact with skin or if inhaled.  
H315: Causes skin irritation.  
H319: Causes serious eye irritation.  
H335: May cause respiratory irritation.

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**Signal words:** Danger

**Hazard pictograms:** GHS02: Flame

GHS06: Skull and crossbones



**Precautionary statements:** P210: Keep away from heat/sparks/open flames/hot surfaces. - No smoking.

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

**Label elements under CHIP:**

**Hazard symbols:** Toxic.



**Risk phrases:** R10: Flammable.

R23/24/25: Toxic by inhalation, in contact with skin and if swallowed.

R36/37/38: Irritating to eyes, respiratory system and skin.

**Safety phrases:** S23: Do not breathe vapour.

S26: In case of contact with eyes, rinse immediately with plenty of water and seek medical advice.

S28: After contact with skin, wash immediately with plenty of water.

S36/37/39: Wear suitable protective clothing, gloves and eye / face protection.

S45: In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible).

### 2.3. Other hazards

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

**PBT:** This substance is not identified as a PBT substance.

## Section 3: Composition/information on ingredients

### 3.1. Substances

**Chemical identity:** 4,4,4-TRIFLUOROBUTANENITRILE

**CAS number:** 690-95-9

## 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. Transfer to hospital if there are burns or symptoms of poisoning.

**Eye contact:** Bathe the eye with running water for 15 minutes. Transfer to hospital for specialist examination.

**Ingestion:** Wash out mouth with water. Do not induce vomiting. If unconscious, check for breathing

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and apply artificial respiration if necessary. If unconscious and breathing is OK, place in the recovery position. Transfer to hospital as soon as possible.

**Inhalation:** Remove casualty from exposure ensuring one's own safety whilst doing so. If conscious, ensure the casualty sits or lies down. If unconscious and breathing is OK, place in the recovery position. If unconscious, check for breathing and apply artificial respiration if necessary. If breathing becomes bubbly, have the casualty sit and provide oxygen if available. Transfer to hospital as soon as possible.

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

**Skin contact:** There may be redness or whiteness of the skin in the area of exposure. Irritation or pain may occur at the site of contact. Absorption through the skin may be fatal.

**Eye contact:** There may be severe pain. The eyes may water profusely.

**Ingestion:** There may be soreness and redness of the mouth and throat. There may be vomiting. Convulsions may occur. There may be loss of consciousness.

**Inhalation:** There may be shortness of breath with a burning sensation in the throat. Absorption through the lungs can occur causing symptoms similar to those of ingestion. Convulsions may occur. There may be loss of consciousness.

**Delayed / immediate effects:** Immediate effects can be expected after short-term exposure.

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

**Immediate / special treatment:** Immediate medical attention is required. Show this safety data sheet to the doctor in attendance.

## Section 5: Fire-fighting measures

### 5.1. Extinguishing media

**Extinguishing media:** Carbon dioxide, dry chemical powder, foam. Use water spray to cool containers.

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

**Exposure hazards:** Flammable. Toxic. Forms explosive air-vapour mixture. In combustion emits toxic fumes of carbon dioxide / carbon monoxide. Nitrogen oxides (NOx). Hydrogen cyanide (HCN). 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:** Notify the police and fire brigade immediately. Eliminate all sources of ignition. 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. Do not attempt to take action without suitable protective

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clothing - see section 8 of SDS. Turn leaking containers leak-side up to prevent the escape of liquid.

**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:** Clean-up should be dealt with only by qualified personnel familiar with the specific substance. 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**

**Reference to other sections:** Refer to section 8 of SDS.

**Section 7: Handling and storage**

**7.1. Precautions for safe handling**

**Handling requirements:** Avoid direct contact with the substance. Ensure there is exhaust ventilation of the area. 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:** Keep container tightly closed. Keep away from sources of ignition. Prevent the build up of electrostatic charge in the immediate area. Ensure lighting and electrical equipment are not a source of ignition. Moisture 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)**

**Specific end use(s):** No data available.

**Section 8: Exposure controls/personal protection**

**8.1. Control parameters**

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

**DNEL / PNEC** No data available.

**8.2. Exposure controls**

**Engineering measures:** Ensure there is exhaust 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 with side-shields. Ensure eye bath is to hand.

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**Skin protection:** Impermeable protective clothing.

**Section 9: Physical and chemical properties**

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

**State:** Clear liquid

**Boiling point/range °C:** 139-140

**Relative density:** 1.21

**9.2. Other information**

**Other information:** No data available.

**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.  
Decomposition may occur on exposure to conditions or materials listed below.

**10.4. Conditions to avoid**

**Conditions to avoid:** Heat. Hot surfaces. Sources of ignition. Flames. Moist air. Humidity.

**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. Nitrogen oxides (NO<sub>x</sub>). Hydrogen cyanide (HCN). Hydrogen fluoride (HF).

**Section 11: Toxicological information**

**11.1. Information on toxicological effects**

**Relevant hazards for substance:**

Hazard	Route	Basis
Acute toxicity (ac. tox. 3)	INH DRM ING	Based on test data
Skin corrosion/irritation	DRM	Based on test data
Serious eye damage/irritation	OPT	Based on test data
STOT-single exposure	INH	Based on test data

**Symptoms / routes of exposure**

**Skin contact:** There may be redness or whiteness of the skin in the area of exposure. Irritation or pain may occur at the site of contact. Absorption through the skin may be fatal.

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**Eye contact:** There may be severe pain. The eyes may water profusely.

**Ingestion:** There may be soreness and redness of the mouth and throat. There may be vomiting.  
Convulsions may occur. There may be loss of consciousness.

**Inhalation:** There may be shortness of breath with a burning sensation in the throat. Absorption through the lungs can occur causing symptoms similar to those of ingestion.  
Convulsions may occur. There may be loss of consciousness.

**Delayed / immediate effects:** Immediate effects can be expected after short-term exposure.

## 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 substance is not identified as a PBT substance.

### 12.6. Other adverse effects

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

## Section 13: Disposal considerations

### 13.1. Waste treatment methods

**Disposal operations:** 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:** UN3273

### 14.2. UN proper shipping name

**Shipping name:** NITRILES, FLAMMABLE, TOXIC, N.O.S.

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**14.3. Transport hazard class(es)**

**Transport class:** 3 (6.1)

**14.4. Packing group**

**Packing group:** II

**14.5. Environmental hazards**

**Environmentally hazardous:** No

**Marine pollutant:** No

**14.6. Special precautions for user**

**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?](http://ecb.jrc.ec.europa.eu/qsar/qsar-tools/index.php?c=TOXTREE)

c=TOXTREE

~ Data predicted using computational software ACD/ToxSuite v 2.95.1 Copyright 1994-2009 ACD/labs, Copyright 2001-2009 Pharma Algorithms, Inc, Advanced Chemistry Development, Inc (ACD/Labs). [http://www.acdlabs.com/products/pc\\_admet/tox/tox/](http://www.acdlabs.com/products/pc_admet/tox/tox/)

**Phrases used in s.2 and 3:** H226: Flammable liquid and vapour.  
H301+311+331: Toxic if swallowed, in contact with skin or if inhaled.  
H315: Causes skin irritation.  
H319: Causes serious eye irritation.  
H335: May cause respiratory irritation.  
R10: Flammable.  
R23/24/25: Toxic by inhalation, in contact with skin and if swallowed.  
R36/37/38: Irritating to eyes, respiratory system and skin.

**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 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

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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.