

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

### 1.1. Product identifier

**Product name:** 4-AMINO-2-(TRIFLUOROMETHYL)BENZONITRILE

**CAS number:** 654-70-6

**Product code:** PC1070L

**Synonyms:** 5-AMINO-2-CYANOBENZOTRIFLUORIDE  
4-CYANO-3-(TRIFLUOROMETHYL)ANILINE

### 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:** T: R23/24/25; Xi: R36/38; Sens.: R43

**Classification under CLP:** Acute Tox. 3: H301+311+331; Eye Irrit. 2: H319; Skin Irrit. 2: H315; Skin Sens. 1: H317

**Most important adverse effects:** Toxic by inhalation, in contact with skin and if swallowed. Irritating to eyes and skin. May cause sensitisation by skin contact.

### 2.2. Label elements

#### Label elements under CLP:

**Hazard statements:** H315: Causes skin irritation.  
H317: May cause an allergic skin reaction.  
H319: Causes serious eye irritation.  
H301+311+331: Toxic if swallowed, in contact with skin or if inhaled.

**Signal words:** Danger

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**Hazard pictograms:** GHS06: Skull and crossbones



**Precautionary statements:** P280: Wear protective gloves/protective clothing/eye protection/face protection.  
P309+311: IF exposed or if you feel unwell: Call a POISON CENTER or doctor.

**Label elements under CHIP:**

**Hazard symbols:** Toxic.



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

R36/38: Irritating to eyes and skin.

R43: May cause sensitisation by skin contact.

**Safety phrases:** S22: Do not breathe dust.

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).

S63: In case of accident by inhalation, remove casualty to fresh air and keep at rest.

## 2.3. Other hazards

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

## Section 3: Composition/information on ingredients

### 3.1. Substances

**Chemical identity:** 4-AMINO-2-(TRIFLUOROMETHYL)BENZONITRILE

## 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 conscious, give half a litre of water to drink immediately. If unconscious, check for breathing and apply artificial respiration if necessary. If unconscious and breathing is OK, place in the recovery position. Transfer to hospital as soon as possible.

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**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. 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:** Toxic. In combustion emits toxic fumes of carbon dioxide / carbon monoxide. Nitrogen oxides (NO<sub>x</sub>). 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. 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 clothing - see section 8 of SDS. Do not create dust.

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## 6.2. Environmental precautions

**Environmental precautions:** Do not discharge into drains or rivers.

## 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. Transfer to a closable, labelled salvage container for disposal by an appropriate method.

## 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 dust in the air. Only use in fume hood.

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

**Storage conditions:** Store in cool, well ventilated area. Keep container tightly closed. Light Sensitive. 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:** Not applicable.

### 8.2. Exposure controls

**Engineering measures:** Ensure there is exhaust ventilation of the area.

**Respiratory protection:** Self-contained breathing apparatus must be available in case of emergency. Particle filter class P1 (EN143).

**Hand protection:** Protective gloves.

**Eye protection:** Safety glasses with side-shields. Ensure eye bath is to hand.

**Skin protection:** Protective clothing.

## Section 9: Physical and chemical properties

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

**State:** Solid

**Colour:** Cream

**Solubility in water:** Insoluble

**Also soluble in:** Methanol. Pyridine.

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Melting point/range °C: 142-144

Part.coeff. n-octanol/water: log Pow: 2.189

## 9.2. Other information

Other information: Not applicable.

## 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.

### 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. Light.

### 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 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
Respiratory/skin sensitisation	DRM	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.

**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.

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

## Section 12: Ecological information

### 12.1. Toxicity

**Ecotoxicity values:** Not applicable.

### 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:** UN3439

### 14.2. UN proper shipping name

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

### 14.3. Transport hazard class(es)

**Transport class:** 6.1

### 14.4. Packing group

**Packing group:** III

### 14.5. Environmental hazards

**Environmentally hazardous:** No

**Marine pollutant:** No

[cont...]

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## 14.6. Special precautions for user

**Special precautions:** No special precautions.

**Tunnel code:** E

**Transport category:** 2

## 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>

~ 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:** H301+311+331: Toxic if swallowed, in contact with skin or if inhaled.  
H315: Causes skin irritation.  
H317: May cause an allergic skin reaction.  
H319: Causes serious eye irritation.  
R23/24/25: Toxic by inhalation, in contact with skin and if swallowed.  
R36/38: Irritating to eyes and skin.  
R43: May cause sensitisation by skin contact.

**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 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.