

3-CYANO-5-NITROBENZOTRIFLUORIDE

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

## 1.1. Product identifier

Product name: 3-CYANO-5-NITROBENZOTRIFLUORIDE

**CAS number:** 20566-80-7

Product code: PC9255

Synonyms: 3-NITRO-5-(TRIFLUOROMETHYL)BENZONITRILE

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

Classification under CLP: Acute Tox. 3: H301+311+331

Most important adverse effects: Toxic by inhalation, in contact with skin and if swallowed.

2.2. Label elements

Label elements:

Hazard statements: H301+311+331: Toxic if swallowed, in contact with skin or if inhaled.

Signal words: Danger

Hazard pictograms: GHS06: Skull and crossbones



Precautionary statements: P260: Do not breathe dust.

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P271: Use only outdoors or in a well-ventilated area.

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

#### Label elements under CHIP:

Hazard symbols: Toxic.



Risk phrases:R23/24/25: Toxic by inhalation, in contact with skin and if swallowed.Safety phrases:S26: In case of contact with eyes, rinse immediately with plenty of water and seek<br/>medical advice.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<br/>the label where possible).

### 2.3. Other hazards

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

### Section 3: Composition/information on ingredients

### 3.1. Substances

Chemical identity: 3-CYANO-5-NITROBENZOTRIFLUORIDE

CAS number: 20566-80-7

#### 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.
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.

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Eye contact:	There may be severe pain. The eyes may water profusely.		I
Ingestion:	There may be soreness and redness of the mouth and throat. There may be vomiting.		I
	Convulsions may occur. There may be loss of consciousness.		I
Inhalation:	There may be shortness of breath with a burning sensation in the throat. Absorption		I
	through the lungs can occur causing symptoms similar to those of ingestion.		I
	Convulsions may occur. There may be loss of consciousness.		I
Delayed / immediate effects:	Immediate effects can be expected after short-term exposure.		I
4.3. Indication of any immediat	e medical attention and special treatment needed		
Immediate / special treatment:	Immediate medical attention is required. Show this safety data sheet to the doctor in		I
	attendance.		I
Section 5: Fire-fighting measured	res		
5.1. Extinguishing media			
	Out the stimulation model for the summarian first should be used. Cothen disvide		
Extinguishing media:	Suitable extinguishing media for the surrounding fire should be used. Carbon dioxide,		
	dry chemical powder, foam.		
5.2. Special hazards arising fro	m the substance or mixture		
Exposure hazards:	Toxic. In combustion emits toxic fumes. Nitrogen oxides (NOx).		
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 n	neasures		
6.1. Personal precautions, prof	tective equipment and emergency procedures		7
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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.		
6.2. Environmental precautions			
6.3. Methods and material for c	Do not discharge into drains or rivers.		
	- ·		
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 section	S		
Reference to other sections:	Refer to section 8 of SDS.		

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#### 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 a cool, well ventilated area. Keep container tightly closed.

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** Values

DNEL / PNEC No data available.

#### 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

### 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.

### 10.3. Possibility of hazardous reactions

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

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#### 10.4. Conditions to avoid

### Conditions to avoid: Heat.

### 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.

#### Section 11: Toxicological information

11.1. Information on toxicological effects

#### **Relevant hazards for product:**

Hazard	Route	Basis
Acute toxicity (ac. tox. 3)	INH DRM ING	Hazardous: calculated

#### 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.

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 product is not identified as a PBT/vPvB substance.

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#### 12.6. Other adverse effects

### Other adverse effects: No data available.

### 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: UN2811

14.2. UN proper shipping name

Shipping name: TOXIC SOLID, ORGANIC, 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

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

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Other information	
Other information:	This safety data sheet is prepared in accordance with Commission Regulation (EU) No 2015/830.
	* Data predicted using computational software. The OECD QSAR-Toolbox for grouping chemicals into categories. Developed by LMC bulgaria.
	http://echa.europa.eu/support/oecd-qsar-toolbox
	~ 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/
Phrases used in s.2 and s.3:	H301+311+331: Toxic if swallowed, in contact with skin or if inhaled.
	R23/24/25: Toxic by inhalation, in contact with skin and if swallowed.
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