

3-Cyano-4-fluorobenzoic acid Apollo Scientific

Part Number: **PC6131** Version No: **1.2** Safety Data Sheet

Chemwatch Hazard Alert Code: 2

Issue Date: **24/05/2023**Print Date: **24/05/2023**S.GHS.GB-NIR.EN

SECTION 1 Identification of the substance / mixture and of the company / undertaking

Product Identifier

Product name	3-Cyano-4-fluorobenzoic acid	
Chemical Name	3-Cyano-4-fluorobenzoic acid	
Synonyms	Not Available	
Other means of identification	Not Available	
CAS number	171050-06-9*	

Relevant identified uses of the substance or mixture and uses advised against

Relevant identified uses Not Available

Details of the manufacturer or supplier of the safety data sheet

Registered company name	Apollo Scientific	Apollo Scientific Itd
Address	Whitefield Road, Bredbury SK62QR United Kingdom	Whitefield Road Not Available SK6 2QR United Kingdom (NI)
Telephone	01614060505	+44(0) 161 406 0505
Fax	0161 406 0506	Not Available
Website	http://www.apolloscientific.co.uk/	apolloscientific.co.uk
Email	sales@apolloscientific.co.uk	sales@apolloscientific.co.uk

Emergency telephone number

Association / Organisation	Not Available
Emergency telephone numbers	Not Available
Other emergency telephone numbers	Not Available

SECTION 2 Hazards identification

Classification of the substance or mixture

Classification according to
regulation (EC) No
1272/2008 [CLP] and
amendments [1]

H312 - Acute Toxicity (Dermal) Category 4, H332 - Acute Toxicity (Inhalation) Category 4, H335 - Specific Target Organ Toxicity - Single Exposure (Respiratory Tract Irritation) Category 3, H302 - Acute Toxicity (Oral) Category 4, H315 - Skin Corrosion/Irritation Category 2, H319 - Serious Eye Damage/Eye Irritation Category 2

Legend: 1. Classified by Chemwatch; 2. Classification drawn from Regulation (EU) No 1272/2008 - Annex VI

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Label elements





Signal word

Warning

Hazard statement(s)

H312	Harmful in contact with skin.
H332	Harmful if inhaled.
H335	May cause respiratory irritation.
H302	Harmful if swallowed.
H315	Causes skin irritation.
H319	Causes serious eye irritation.

Precautionary statement(s) Prevention

P271	1 Use only outdoors or in a well-ventilated area.	
P261 Avoid breathing dust/fumes.		
P264 Wash all exposed external body areas thoroughly after handling.		
P270 Do not eat, drink or smoke when using this product.		
P280 Wear protective gloves, protective clothing, eye protection and face protection.		

Precautionary statement(s) Response

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Contact lenses, if present lenses, if p		
P302+P352	IF ON SKIN: Wash with plenty of water.	
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.		
P330	Rinse mouth.	
P332+P313	If skin irritation occurs: Get medical advice/attention.	
P362+P364	Take off contaminated clothing and wash it before reuse.	

Precautionary statement(s) Storage

	P405	Store locked up.
	P403+P233	Store in a well-ventilated place. Keep container tightly closed.

Precautionary statement(s) Disposal

P501 Dispose of contents/container to authorised hazardous or special waste collection point in accordance with any local regulation.

SECTION 3 Composition / information on ingredients

Substances

CAS No	%[weight]	Name	Classification according to regulation (EC) No 1272/2008 [CLP] and amendments	SCL / M-Factor
Not Available	100	3-Cyano- 4-fluorobenzoic acid	Acute Toxicity (Dermal) Category 4, Acute Toxicity (Inhalation) Category 4, Specific Target Organ Toxicity - Single Exposure (Respiratory Tract Irritation) Category 3, Acute Toxicity (Oral) Category 4, Skin Corrosion/Irritation Category 2, Serious Eye Damage/Eye Irritation Category 2; H312, H332, H335, H302, H315, H319 [1]	Not Available

Legend:

1. Classified by Chemwatch; 2. Classification drawn from Regulation (EU) No 1272/2008 - Annex VI; 3. Classification drawn from C&L; * EU IOELVs available; [e] Substance identified as having endocrine disrupting properties

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See section above for composition of Substances

SECTION 4 First aid measures

Description of first aid measures

Eye Contact	If this product comes in contact with the eyes: • Wash out immediately with fresh running water. • Ensure complete irrigation of the eye by keeping eyelids apart and away from eye and moving the eyelids by occasionally lifting the upper and lower lids. • Seek medical attention without delay; if pain persists or recurs seek medical attention. • Removal of contact lenses after an eye injury should only be undertaken by skilled personnel.
Skin Contact	If skin or hair contact occurs: Flush skin and hair with running water (and soap if available). Seek medical attention in event of irritation.
Inhalation	 If fumes, aerosols or combustion products are inhaled remove from contaminated area. Other measures are usually unnecessary.
Ingestion	 Immediately give a glass of water. First aid is not generally required. If in doubt, contact a Poisons Information Centre or a doctor.

Indication of any immediate medical attention and special treatment needed

Treat symptomatically.

SECTION 5 Firefighting measures

Extinguishing media

- ▶ There is no restriction on the type of extinguisher which may be used.
- Use extinguishing media suitable for surrounding area.

Special hazards arising from the substrate or mixture

	Fire Incompatibility	None known.		
Advice for firefighters				
	Fire Fighting	 Alert Fire Brigade and tell them location and nature of hazard. Wear breathing apparatus plus protective gloves in the event of a fire. Prevent, by any means available, spillage from entering drains or water courses. Use fire fighting procedures suitable for surrounding area. DO NOT approach containers suspected to be hot. Cool fire exposed containers with water spray from a protected location. If safe to do so, remove containers from path of fire. Equipment should be thoroughly decontaminated after use. 		
	Fire/Explosion Hazard	 Non combustible. Not considered a significant fire risk, however containers may burn. May emit corrosive fumes. 		

SECTION 6 Accidental release measures

Personal precautions, protective equipment and emergency procedures

See section 8

Environmental precautions

See section 12

Methods and material for containment and cleaning up

Minor Spills	 Clean up all spills immediately. Avoid breathing vapours/ aerosols or dusts and avoid contact with skin and eyes. Place in a suitable, labelled container for waste disposal.
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Minor hazard.

- Clear area of personnel.
- ▶ Alert Fire Brigade and tell them location and nature of hazard.
- ▶ Control personal contact with the substance, by using protective equipment as required.
- Prevent spillage from entering drains or water ways.
- ▶ Contain spill with sand, earth or vermiculite.
- ▶ Collect recoverable product into labelled containers for recycling.
- Absorb remaining product with sand, earth or vermiculite and place in appropriate containers for disposal.
- Wash area and prevent runoff into drains or waterways.
- If contamination of drains or waterways occurs, advise emergency services.

Personal Protective Equipment advice is contained in Section 8 of the SDS.

SECTION 7 Handling and storage

Major Spills

Precautions for safe handling

- Avoid all personal contact, including inhalation.
- Wear protective clothing when risk of exposure occurs.
- ▶ Use in a well-ventilated area.
- ▶ Prevent concentration in hollows and sumps.
- ▶ DO NOT enter confined spaces until atmosphere has been checked.
- ▶ DO NOT allow material to contact humans, exposed food or food utensils.
- Avoid contact with incompatible materials.
- Safe handling When handling, DO NOT eat, drink or smoke.
 - ▶ Keep containers securely sealed when not in use.
 - Avoid physical damage to containers.
 - Always wash hands with soap and water after handling.
 - Work clothes should be laundered separately. Launder contaminated clothing before re-use.
 - Use good occupational work practice.
 - ▶ Observe manufacturer's storage and handling recommendations contained within this SDS.
 - Atmosphere should be regularly checked against established exposure standards to ensure safe working conditions are maintained.

Other information

Conditions for safe storage, including any incompatibilities

Suitable container

- ▶ Polyethylene or polypropylene container.
- ▶ Packing as recommended by manufacturer.
- ▶ Check all containers are clearly labelled and free from leaks.

Storage incompatibility

None known

SECTION 8 Exposure controls / personal protection

Control parameters

Occupational Exposure Limits (OEL)

INGREDIENT DATA

Not Available

Emergency Limits

Ingredient	TEEL-1	TEEL-2	TEEL-3
3-Cyano-4-fluorobenzoic acid	Not Available	Not Available	Not Available

Ingredient	Original IDLH	Revised IDLH
3-Cyano-4-fluorobenzoic acid	Not Available	Not Available

Exposure controls

Appropriate engineering controls

Engineering controls are used to remove a hazard or place a barrier between the worker and the hazard. Well-designed engineering controls can be highly effective in protecting workers and will typically be independent of worker interactions to provide this high level of protection.

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The basic types of engineering controls are:

Process controls which involve changing the way a job activity or process is done to reduce the risk.

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Enclosure and/or isolation of emission source which keeps a selected hazard "physically" away from the worker and ventilation that strategically "adds" and "removes" air in the work environment. Ventilation can remove or dilute an air contaminant if designed properly. The design of a ventilation system must match the particular process and chemical or contaminant in use. Employers may need to use multiple types of controls to prevent employee overexposure.

General exhaust is adequate under normal operating conditions. Local exhaust ventilation may be required in specific circumstances. If risk of overexposure exists, wear approved respirator. Correct fit is essential to obtain adequate protection. Provide adequate ventilation in warehouse or closed storage areas. Air contaminants generated in the workplace possess varying "escape" velocities which, in turn, determine the "capture velocities" of fresh circulating air required to effectively remove the contaminant.

Type of Contaminant:	Air Speed:
solvent, vapours, degreasing etc., evaporating from tank (in still air).	0.25-0.5 m/s (50-100 f/min)
aerosols, fumes from pouring operations, intermittent container filling, low speed conveyer transfers, welding, spray drift, plating acid fumes, pickling (released at low velocity into zone of active generation)	0.5-1 m/s (100-200 f/min.)
direct spray, spray painting in shallow booths, drum filling, conveyer loading, crusher dusts, gas discharge (active generation into zone of rapid air motion)	1-2.5 m/s (200-500 f/min.)
grinding, abrasive blasting, tumbling, high speed wheel generated dusts (released at high initial velocity into zone of very high rapid air motion).	2.5-10 m/s (500-2000 f/min.)

Within each range the appropriate value depends on:

Lower end of the range	Upper end of the range
1: Room air currents minimal or favourable to capture	1: Disturbing room air currents
2: Contaminants of low toxicity or of nuisance value only.	2: Contaminants of high toxicity
3: Intermittent, low production.	3: High production, heavy use
4: Large hood or large air mass in motion	4: Small hood-local control only

Simple theory shows that air velocity falls rapidly with distance away from the opening of a simple extraction pipe. Velocity generally decreases with the square of distance from the extraction point (in simple cases). Therefore the air speed at the extraction point should be adjusted, accordingly, after reference to distance from the contaminating source. The air velocity at the extraction fan, for example, should be a minimum of 1-2 m/s (200-400 f/min) for extraction of solvents generated in a tank 2 meters distant from the extraction point. Other mechanical considerations, producing performance deficits within the extraction apparatus, make it essential that theoretical air velocities are multiplied by factors of 10 or more when extraction systems are installed or used.

Individual protection measures, such as personal protective equipment











Eye and face protection

- Safety glasses with side shields.
- Chemical goggles.
- Contact lenses may pose a special hazard; soft contact lenses may absorb and concentrate irritants. A written policy document, describing the wearing of lenses or restrictions on use, should be created for each workplace or task. This should include a review of lens absorption and adsorption for the class of chemicals in use and an account of injury experience. Medical and first-aid personnel should be trained in their removal and suitable equipment should be readily available. In the event of chemical exposure, begin eye irrigation immediately and remove contact lens as soon as practicable. Lens should be removed at the first signs of eye redness or irritation - lens should be removed in a clean environment only after workers have washed hands thoroughly. [CDC NIOSH Current Intelligence Bulletin 59], [AS/NZS 1336 or national equivalent]

Skin protection See Hand protection below Wear chemical protective gloves, e.g. PVC. Hands/feet protection Wear safety footwear or safety gumboots, e.g. Rubber **Body protection** See Other protection below Overalls.

Other protection

- P.V.C apron.
- ▶ Barrier cream.
- Skin cleansing cream.
- Eve wash unit.

Respiratory protection

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Required Minimum Protection Factor	Half-Face Respirator	Full-Face Respirator	Powered Air Respirator
up to 10 x ES	P1 Air-line*	-	PAPR-P1
up to 50 x ES	Air-line**	P2	PAPR-P2
up to 100 x ES	-	P3	-
		Air-line*	-
100+ x ES	-	Air-line**	PAPR-P3

 $^{^{\}star}$ - Negative pressure demand ** - Continuous flow

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A(All classes) = Organic vapours, B AUS or B1 = Acid gasses, B2 = Acid gas or hydrogen cyanide(HCN), B3 = Acid gas or hydrogen cyanide(HCN), E = Sulfur dioxide(SO2), G = Agricultural chemicals, K = Ammonia(NH3), Hg = Mercury, NO = Oxides of nitrogen, MB = Methyl bromide, AX = Low boiling point organic compounds(below 65 degC)

SECTION 9 Physical and chemical properties

Information on basic physical and chemical properties

Appearance	Not Available		
Physical state	Powder	Relative density (Water = 1)	Not Available
Odour	Not Available	Partition coefficient n-octanol / water	Not Available
Odour threshold	Not Available	Auto-ignition temperature (°C)	Not Available
pH (as supplied)	Not Available	Decomposition temperature (°C)	Not Available
Melting point / freezing point (°C)	187-188	Viscosity (cSt)	Not Available
Initial boiling point and boiling range (°C)	Not Available	Molecular weight (g/mol)	Not Available
Flash point (°C)	Not Available	Taste	Not Available
Evaporation rate	Not Available	Explosive properties	Not Available
Flammability	Not Available	Oxidising properties	Not Available
Upper Explosive Limit (%)	Not Available	Surface Tension (dyn/cm or mN/m)	Not Available
Lower Explosive Limit (%)	Not Available	Volatile Component (%vol)	Not Available
Vapour pressure (kPa)	Not Available	Gas group	Not Available
Solubility in water	Not Available	pH as a solution (1%)	Not Available
Vapour density (Air = 1)	Not Available	VOC g/L	Not Available

SECTION 10 Stability and reactivity

Reactivity	See section 7
Chemical stability	Product is considered stable and hazardous polymerisation will not occur.
Possibility of hazardous reactions	See section 7
Conditions to avoid	See section 7
Incompatible materials	See section 7
Hazardous decomposition products	See section 5

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SECTION 11 Toxicological information

Information on toxicological effects

Inhaled	The material is not thought to produce adverse health effects or irritation of the respiratory tract (as classified by EC Directives using animal models). Nevertheless, good hygiene practice requires that exposure be kept to a minimum and that suitable control measures be used in an occupational setting.
Ingestion	The material has NOT been classified by EC Directives or other classification systems as "harmful by ingestion". This is because of the lack of corroborating animal or human evidence.
Skin Contact	The material is not thought to produce adverse health effects or skin irritation following contact (as classified by EC Directives using animal models). Nevertheless, good hygiene practice requires that exposure be kept to a minimum and that suitable gloves be used in an occupational setting.
Eye	This material can cause eye irritation and damage in some persons.
Chronic	Long-term exposure to the product is not thought to produce chronic effects adverse to the health (as classified by EC Directives using animal models); nevertheless exposure by all routes should be minimised as a matter of course.
Legend:	1. Value obtained from Europe ECHA Registered Substances - Acute toxicity 2. Value obtained from manufacturer's SDS.

Unless otherwise specified data extracted from RTECS - Register of Toxic Effect of chemical Substances

Acute Toxicity	✓	Carcinogenicity	×
Skin Irritation/Corrosion	✓	Reproductivity	×
Serious Eye Damage/Irritation	✓	STOT - Single Exposure	~
Respiratory or Skin sensitisation	×	STOT - Repeated Exposure	×
Mutagenicity	×	Aspiration Hazard	×

Legend:

🗶 – Data either not available or does not fill the criteria for classification

Data available to make classification

SECTION 12 Ecological information

Toxicity

Legend:

Extracted from 1. IUCLID Toxicity Data 2. Europe ECHA Registered Substances - Ecotoxicological Information - Aquatic Toxicity 4. US EPA, Ecotox database - Aquatic Toxicity Data 5. ECETOC Aquatic Hazard Assessment Data 6. NITE (Japan) -Bioconcentration Data 7. METI (Japan) - Bioconcentration Data 8. Vendor Data

Persistence and degradability

Ingredient	Persistence: Water/Soil	Persistence: Air
	No Data available for all ingredients	No Data available for all ingredients

Bioaccumulative potential

Ingredient	Bioaccumulation
	No Data available for all ingredients

Mobility in soil

Ingredient	Mobility
	No Data available for all ingredients

SECTION 13 Disposal considerations

Waste treatment methods

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Product / Packaging disposal

▶ Recycle wherever possible or consult manufacturer for recycling options.

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- ▶ Consult State Land Waste Management Authority for disposal.
- ▶ Bury residue in an authorised landfill.
- ▶ Recycle containers if possible, or dispose of in an authorised landfill.

SECTION 14 Transport information

Labels Required

Marine Pollutant

NO

Land transport (ADR): NOT REGULATED FOR TRANSPORT OF DANGEROUS GOODS

Air transport (ICAO-IATA / DGR): NOT REGULATED FOR TRANSPORT OF DANGEROUS GOODS

Sea transport (IMDG-Code / GGVSee): NOT REGULATED FOR TRANSPORT OF DANGEROUS GOODS

Inland waterways transport (ADN): NOT REGULATED FOR TRANSPORT OF DANGEROUS GOODS

Transport in bulk according to Annex II of MARPOL and the IBC code

Not Applicable

Transport in bulk in accordance with MARPOL Annex V and the IMSBC Code

Product name	Group
3-Cyano-4-fluorobenzoic acid	Not Available

Transport in bulk in accordance with the IGC Code

Product name	Ship Type
3-Cyano-4-fluorobenzoic acid	Not Available

SECTION 15 Regulatory information

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

National Inventory Status

National Inventory	Status	
Australia - AIIC / Australia Non-Industrial Use	No (3-Cyano-4-fluorobenzoic acid)	
Canada - DSL	No (3-Cyano-4-fluorobenzoic acid)	
Canada - NDSL	No (3-Cyano-4-fluorobenzoic acid)	
China - IECSC	No (3-Cyano-4-fluorobenzoic acid)	
Europe - EINEC / ELINCS / NLP	No (3-Cyano-4-fluorobenzoic acid)	
Japan - ENCS	No (3-Cyano-4-fluorobenzoic acid)	
Korea - KECI	No (3-Cyano-4-fluorobenzoic acid)	
New Zealand - NZIoC	No (3-Cyano-4-fluorobenzoic acid)	
Philippines - PICCS	No (3-Cyano-4-fluorobenzoic acid)	
USA - TSCA	No (3-Cyano-4-fluorobenzoic acid)	
Taiwan - TCSI	No (3-Cyano-4-fluorobenzoic acid)	
Mexico - INSQ	No (3-Cyano-4-fluorobenzoic acid)	
Vietnam - NCI	No (3-Cyano-4-fluorobenzoic acid)	
Russia - FBEPH	No (3-Cyano-4-fluorobenzoic acid)	
Legend:	Yes = All CAS declared ingredients are on the inventory No = One or more of the CAS listed ingredients are not on the inventory. These ingredients may be exempt or will require registration.	

SECTION 16 Other information

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Revision Date	24/05/2023
Initial Date	24/05/2023

SDS Version Summary

Version	Date of Update	Sections Updated
0.2	24/05/2023	Hazards identification - Classification, Composition / information on ingredients - Ingredients, Identification of the substance / mixture and of the company / undertaking - Supplier Information

Other information

Classification of the preparation and its individual components has drawn on official and authoritative sources as well as independent review by the Chemwatch Classification committee using available literature references.

The SDS is a Hazard Communication tool and should be used to assist in the Risk Assessment. Many factors determine whether the reported Hazards are Risks in the workplace or other settings. Risks may be determined by reference to Exposures Scenarios. Scale of use, frequency of use and current or available engineering controls must be considered.

For detailed advice on Personal Protective Equipment, refer to the following EU CEN Standards:

EN 166 Personal eye-protection

EN 340 Protective clothing

EN 374 Protective gloves against chemicals and micro-organisms

EN 13832 Footwear protecting against chemicals

EN 133 Respiratory protective devices

Definitions and abbreviations

PC—TWA: Permissible Concentration-Time Weighted Average PC—STEL: Permissible Concentration-Short Term Exposure Limit

IARC: International Agency for Research on Cancer

ACGIH: American Conference of Governmental Industrial Hygienists

STEL: Short Term Exposure Limit

TEEL: Temporary Emergency Exposure Limit。

IDLH: Immediately Dangerous to Life or Health Concentrations

ES: Exposure Standard
OSF: Odour Safety Factor

NOAEL :No Observed Adverse Effect Level LOAEL: Lowest Observed Adverse Effect Level

TLV: Threshold Limit Value LOD: Limit Of Detection OTV: Odour Threshold Value BCF: BioConcentration Factors BEI: Biological Exposure Index

AIIC: Australian Inventory of Industrial Chemicals

DSL: Domestic Substances List NDSL: Non-Domestic Substances List

IECSC: Inventory of Existing Chemical Substance in China

EINECS: European INventory of Existing Commercial chemical Substances

ELINCS: European List of Notified Chemical Substances

NLP: No-Longer Polymers

ENCS: Existing and New Chemical Substances Inventory

KECI: Korea Existing Chemicals Inventory NZIoC: New Zealand Inventory of Chemicals

PICCS: Philippine Inventory of Chemicals and Chemical Substances

TSCA: Toxic Substances Control Act
TCSI: Taiwan Chemical Substance Inventory
INSQ: Inventario Nacional de Sustancias Químicas

NCI: National Chemical Inventory

FBEPH: Russian Register of Potentially Hazardous Chemical and Biological Substances

Classification and procedure used to derive the classification for mixtures according to Regulation (EC) 1272/2008 [CLP]

Classification according to regulation (EC) No 1272/2008 [CLP] and amendments	Classification Procedure
Acute Toxicity (Dermal) Category 4, H312	Expert judgement
Acute Toxicity (Inhalation) Category 4, H332	Expert judgement

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Classification according to regulation (EC) No 1272/2008 [CLP] and amendments	Classification Procedure
Specific Target Organ Toxicity - Single Exposure (Respiratory Tract Irritation) Category 3 , H335	Expert judgement
Acute Toxicity (Oral) Category 4, H302	Expert judgement
Skin Corrosion/Irritation Category 2, H315	Expert judgement
Serious Eye Damage/Eye Irritation Category 2, H319	Expert judgement

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