

2,3,6-TRIFLUOROPHENYLACETONITRILE

Page: 1

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

1.1. Product identifier

Product name: 2,3,6-TRIFLUOROPHENYLACETONITRILE

CAS number: 114152-21-5 Product code: PC7818L

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: R37

Classification under CLP: Acute Tox. 3: H301+311+331; STOT SE 3: H335

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

2.2. Label elements

Label elements under CLP:

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

H335: May cause respiratory irritation.

Signal words: Danger

Hazard pictograms: GHS06: Skull and crossbones



Precautionary statements: P260: Do not breathe vapours.

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

P312: Call a POISON CENTER or doctor if you feel unwell.

2,3,6-TRIFLUOROPHENYLACETONITRILE

Page: 2

Label elements under CHIP:

Hazard symbols: Toxic.



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

R37: Irritating to respiratory system.

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: 2,3,6-TRIFLUOROPHENYLACETONITRILE

CAS number: 114152-21-5

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

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.

2,3,6-TRIFLUOROPHENYLACETONITRILE

Page: 3

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: Toxic. 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. 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. 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.

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 exhaust ventilation of the area.

Avoid the formation or spread of mists 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.

Suitable packaging: Must only be kept in original packaging.

2,3,6-TRIFLUOROPHENYLACETONITRILE

Page: 4

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.

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.

Skin protection: Impermeable protective clothing.

Section 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

State: Liquid

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.

10.4. Conditions to avoid

Conditions to avoid: Heat. Hot surfaces. Flames.

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

(NOx). Hydrogen cyanide (HCN). Hydrogen fluoride (HF).

2,3,6-TRIFLUOROPHENYLACETONITRILE

Page: 5

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
Acute toxicity (ac. tox. 2)	-	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.

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.

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.

[cont...]

2,3,6-TRIFLUOROPHENYLACETONITRILE

Page: 6

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: UN3276

14.2. UN proper shipping name

Shipping name: NITRILES, LIQUID, TOXIC, 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

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.

* 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/

Phrases used in s.2 and 3: H301+311+331: Toxic if swallowed, in contact with skin or if inhaled.

H335: May cause respiratory irritation.

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

R37: Irritating to respiratory system.

2,3,6-TRIFLUOROPHENYLACETONITRILE

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Page: 7