-5-BROMO-2-METHYL-3-(TRIFLUOROMETHYL)BENZONITRILE

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

1.1. Product identifier

Product name: 5-BROMO-2-METHYL-3-(TRIFLUOROMETHYL)BENZONITRILE

CAS number: 2387259-19-8 Product code: PC303595

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

Supporting Discovery

Company name: Apollo Scientific Itd

Units 3 & 4 Parkway Denton Manchester M34 3SG UK

Tel: 01616411420

Email: alan.myers@apolloscientific.co.uk

1.4. Emergency telephone number

Emergency tel: -

Section 2: Hazards identification

2.1. Classification of the substance or mixture

Classification under CLP: Acute Tox. 3: H311; Acute Tox. 4: H302+H332; Eye Irrit. 2: H319; Skin Irrit. 2: H315

Most important adverse effects: Harmful if swallowed or if inhaled Toxic in contact with skin. Causes skin irritation.

Causes serious eye irritation.

2.2. Label elements

Label elements:

Hazard statements: H302+H332: Harmful if swallowed or if inhaled

H311: Toxic in contact with skin. H315: Causes skin irritation.

H319: Causes serious eye irritation.

Hazard pictograms: GHS06: Skull and crossbones



Signal words: Danger

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

P301+P312: IF SWALLOWED: Call a POISON CENTER if you feel unwell.

P361+P364: Take off immediately all contaminated clothing and wash it before reuse.

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: 5-BROMO-2-METHYL-3-(TRIFLUOROMETHYL)BENZONITRILE

CAS number: 2387259-19-8

Section 4: First aid measures

4.1. Description of first aid measures

Skin contact: Wash immediately with plenty of soap and water.

Eye contact: Bathe the eye with running water for 15 minutes.

Ingestion: Do not induce vomiting. Wash out mouth with water. If conscious, give half a litre of water

to drink immediately. Transfer to hospital as soon as possible.

Inhalation: Remove casualty from exposure ensuring one's own safety whilst doing so. Consult a

doctor.

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

Skin contact: There may be irritation and redness at the site of contact.

Eye contact: There may be irritation and redness. The eyes may water profusely.

Ingestion: There may be soreness and redness of the mouth and throat. Nausea and stomach

pain may occur. There may be vomiting.

Inhalation: There may be irritation of the throat with a feeling of tightness in the chest.

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.

5.2. Special hazards arising from the substance or mixture

Exposure hazards: In combustion emits toxic fumes of carbon dioxide / carbon monoxide. Nitrogen oxides

(NOx). Hydrogen bromide (HBr). 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. Keep cylinders cool with water spray.

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Section 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

Personal precautions: Refer to section 8 of SDS for personal protection details. 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.

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: Transfer to a closable, labelled salvage container for disposal by an appropriate

method. Avoid all incompatible materials in clean-up procedure - see section 10 of SDS.

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 sufficient ventilation of the area.

Do not handle in a confined space. 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)

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 sufficient ventilation of the area.

Respiratory protection: Self-contained breathing apparatus must be available in case of emergency. Respiratory

protective device with particle filter.

Hand protection: Protective gloves.

Eye protection: Safety glasses. Ensure eye bath is to hand.

Skin protection: Protective clothing.

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Section 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

State: Solid

Evaporation rate: No data available.

Oxidising: No data available.

Solubility in water: No data available.

Viscosity: No data available.

Boiling point/range °C: No data available. Melting point/range °C: No data available.

Flammability limits %: lower: No data available. upper: No data available.

Flash point °C: No data available. Part.coeff. n-octanol/water: No data available.

Autoflammability°C: No data available. Vapour pressure: No data available.

Relative density: No data available. pH: No data available.

VOC g/I: No data available.

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.

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 fluoride (HF). Hydrogen bromide gas (HBr).

Section 11: Toxicological information

11.1. Information on toxicological effects

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Relevant hazards for product:

Hazard	Route	Basis
Acute toxicity (ac. tox. 4)	INH ING	Hazardous: calculated
Acute toxicity (ac. tox. 3)	DRM	Hazardous: calculated
Skin corrosion/irritation	DRM	Hazardous: calculated
Serious eye damage/irritation	OPT	Hazardous: calculated

Symptoms / routes of exposure

Skin contact: There may be irritation and redness at the site of contact.

Eye contact: There may be irritation and redness. The eyes may water profusely.

Ingestion: There may be soreness and redness of the mouth and throat. Nausea and stomach

pain may occur. There may be vomiting.

Inhalation: There may be irritation of the throat with a feeling of tightness in the chest.

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.

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.

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Section 14: Transport information

14.1. UN number

UN number: UN3439

14.2. UN proper shipping name

Shipping name: NITRILES, SOLID, 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

Specific regulations: Not applicable.

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

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: H302+H332: Harmful if swallowed or if inhaled

H311: Toxic in contact with skin.

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