

SAFETY DATA SHEET

3-[3-(TRIFLUOROMETHYL)PHENYL]PROPAN-1-OL

Page: 1

Compilation date: 06/02/2012

Revision No: 1

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

1.1. Product identifier

Product name: 3-[3-(TRIFLUOROMETHYL)PHENYL]PROPAN-1-OL

CAS number: 78573-45-2

Product code: PC57025

Synonyms: 3-(3-HYDROXYPROP-1-YL)BENZOTRIFLUORIDE

3-(3-HYDROXYPROP-1-YL)-ALPHA,ALPHA,ALPHA-TRIFLUOROTOLUENE

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: Xi: R38; Xi: R41; -: R52/53

Classification under CLP: Eye Dam. 1: H318; Aquatic Chronic 3: H412; Skin Irrit. 2: H315

Most important adverse effects: Irritating to skin. Risk of serious damage to eyes. Harmful to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

2.2. Label elements

Label elements under CLP:

Hazard statements: H315: Causes skin irritation.

H318: Causes serious eye damage.

H412: Harmful to aquatic life with long lasting effects.

Signal words: Danger

Hazard pictograms: GHS05: Corrosion



SAFETY DATA SHEET

3-[3-(TRIFLUOROMETHYL)PHENYL]PROPAN-1-OL

Page: 2

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: Irritant.



Risk phrases: R38: Irritating to skin.
R41: Risk of serious damage to eyes.
R52/53: Harmful to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

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: 3-[3-(TRIFLUOROMETHYL)PHENYL]PROPAN-1-OL

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. Wash immediately with plenty of soap and water.

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. Consult a doctor.

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

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 pain and redness. The eyes may water profusely. There may be severe pain. The vision may become blurred. May cause permanent damage.

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

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

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: Eye bathing equipment should be available on the premises.

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SAFETY DATA SHEET

3-[3-(TRIFLUOROMETHYL)PHENYL]PROPAN-1-OL

Page: 3

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: In combustion emits toxic fumes of carbon dioxide / carbon monoxide. 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: 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: 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

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 sufficient 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. 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.

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SAFETY DATA SHEET

3-[3-(TRIFLUOROMETHYL)PHENYL]PROPAN-1-OL

Page: 4

Section 8: Exposure controls/personal protection

8.1. Control parameters

Workplace exposure limits: Not applicable.

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.

Hand protection: Protective gloves.

Eye protection: Tightly fitting safety goggles. 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: Liquid

Colour: Pale yellow

Solubility in water: Not miscible

Also soluble in: Dichloromethane. Ethyl acetate.

Boiling point/range °C: 68-71/0.4mmHg

Part.coeff. n-octanol/water: log Pow 3.02

Relative density: 1.1

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.

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. Hydrogen fluoride (HF).

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SAFETY DATA SHEET

3-[3-(TRIFLUOROMETHYL)PHENYL]PROPAN-1-OL

Page: 5

Section 11: Toxicological information

11.1. Information on toxicological effects

Relevant hazards for substance:

Hazard	Route	Basis
Skin corrosion/irritation	DRM	Based on test data
Serious eye damage/irritation	OPT	Based on test data

Symptoms / routes of exposure

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

Eye contact: There may be pain and redness. The eyes may water profusely. There may be severe pain. The vision may become blurred. May cause permanent damage.

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

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

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: Not readily biodegradable (The statement has been derived from the structure of the product)

12.3. Bioaccumulative potential

Bioaccumulative potential: Because of the n-octanol/water distribution coefficient (log Pow) accumulation in organisms is possible

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: LC50 (96 h) 17 mg/l, Fish (calculated) EC50 (48 h) 19 mg/l, daphnia (calculated) EC50 (96 h) 13 mg/l, algae (calculated) The product has not been tested. The statements have been derived from the structure of the product.

Section 13: Disposal considerations

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SAFETY DATA SHEET

3-[3-(TRIFLUOROMETHYL)PHENYL]PROPAN-1-OL

Page: 6

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

Transport class: This product does not require a classification for transport.

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: H315: Causes skin irritation.
H318: Causes serious eye damage.
H412: Harmful to aquatic life with long lasting effects.
R38: Irritating to skin.

R41: Risk of serious damage to eyes.

R52/53: Harmful to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

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

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SAFETY DATA SHEET

3-[3-(TRIFLUOROMETHYL)PHENYL]PROPAN-1-OL

Page: 7

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.