

SAFETY DATA SHEET

3-FLUORO-4-(METHYLSULPHONYL)BENZOIC ACID

Page: 1

Compilation date: 29/07/2010

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Revision No: 3

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

1.1. Product identifier

Product name: 3-FLUORO-4-(METHYLSULPHONYL)BENZOIC ACID

CAS number: 185945-88-4

Product code: PC7551

Synonyms: 4-CARBOXY-3-FLUOROPHENYL METHYL SULPHONE

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 CLP: STOT SE 3: H335; Eye Irrit. 2: H319; Skin Irrit. 2: H315

Most important adverse effects: Causes skin irritation. Causes serious eye irritation. May cause respiratory irritation.

2.2. Label elements

Label elements:

Hazard statements: H315: Causes skin irritation.

H319: Causes serious eye irritation.

H335: May cause respiratory irritation.

Signal words: Warning

Hazard pictograms: GHS07: Exclamation mark



SAFETY DATA SHEET

3-FLUORO-4-(METHYLSULPHONYL)BENZOIC ACID

Page: 2

Precautionary statements: P271: Use only outdoors or in a well-ventilated area.
P261: Avoid breathing dust.
P280: Wear protective gloves/protective clothing/eye protection/face protection.

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-FLUORO-4-(METHYLSULPHONYL)BENZOIC ACID

CAS number: 185945-88-4

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. Consult a doctor.

Ingestion: Wash out mouth with water. Consult a doctor.

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.

Inhalation: There may be irritation of the throat with a feeling of tightness in the chest. Exposure may cause coughing or wheezing.

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. Sulphur oxides (SO_x). 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.

[cont...]

SAFETY DATA SHEET

3-FLUORO-4-(METHYLSULPHONYL)BENZOIC ACID

Page: 3

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. Do not create dust.

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.

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. Air sensitive. Store under Argon.

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 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.

[cont...]

SAFETY DATA SHEET

3-FLUORO-4-(METHYLSULPHONYL)BENZOIC ACID

Page: 4

Skin protection: Protective clothing.

Section 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

State: Powder

Colour: White

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.

Flammability limits %: lower: No data available.

Flash point °C: No data available.

Autoflammability °C: No data available.

Relative density: No data available.

VOC g/l: No data available.

Melting point/range °C: 212-213

upper: No data available.

Part.coeff. n-octanol/water: No data available.

Vapour pressure: No data available.

pH: 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. Air.

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). Sulphur oxides (SOx)

Section 11: Toxicological information

11.1. Information on toxicological effects

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SAFETY DATA SHEET

3-FLUORO-4-(METHYLSULPHONYL)BENZOIC ACID

Page: 5

Relevant hazards for product:

Hazard	Route	Basis
Skin corrosion/irritation	DRM	Hazardous: calculated
Serious eye damage/irritation	OPT	Hazardous: calculated
STOT-single exposure	INH	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.

Inhalation: There may be irritation of the throat with a feeling of tightness in the chest. Exposure may cause coughing or wheezing.

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: 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.

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SAFETY DATA SHEET

3-FLUORO-4-(METHYLSULPHONYL)BENZOIC ACID

Page: 6

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 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/oeqd-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: H315: Causes skin irritation.

H319: Causes serious eye irritation.

H335: May cause respiratory irritation.

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 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.