

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

1.1. Product identifier

Product name: 4-METHYLPHENYLSULPHUR PENTAFLUORIDE
CAS number: 203126-21-0
Product code: PC49104
Synonyms: 4-(PENTAFLUOROTHIO)TOLUENE
4-(PENTAFLUOROSULPHANYL)TOLUENE
1-METHYL-4-(PENTAFLUOROSULPHANYL)BENZENE

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: R25; Xi: R36/38
Classification under CLP: Acute Tox. 3: H301; Eye Irrit. 2: H319; Skin Irrit. 2: H315
Most important adverse effects: Toxic if swallowed. Irritating to eyes and skin.

2.2. Label elements

Label elements under CLP:

Hazard statements: H301: Toxic if swallowed.
H315: Causes skin irritation.
H319: Causes serious eye irritation.
Signal words: Danger
Hazard pictograms: GHS06: Skull and crossbones
GHS07: Exclamation mark

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Precautionary statements: P261: Avoid breathing vapours.
P280: Wear protective gloves/protective clothing/eye protection.
P312: Call a POISON CENTER or doctor if you feel unwell.

Label elements under CHIP:

Hazard symbols: Toxic.



Risk phrases: R25: Toxic if swallowed.
R36/38: Irritating to eyes and skin.

Safety phrases: S16: Keep away from sources of ignition - No smoking.
S36/37/39: Wear suitable protective clothing, gloves and eye / face protection.
S45: In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible).

2.3. Other hazards

Other hazards: Combustible (H227)

PBT: This substance is not identified as a PBT substance.

Section 3: Composition/information on ingredients

3.1. Substances

Chemical identity: 4-METHYLPHENYLSULPHUR PENTAFLUORIDE

CAS number: 203126-21-0

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. Consult a doctor.

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

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. Transfer to hospital as soon as possible.

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.

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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.

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: Immediate medical attention is required. Show this safety data sheet to the doctor in attendance.

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. 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.

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 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

Reference to other sections: Refer to section 8 of SDS.

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Section 7: Handling and storage

7.1. Precautions for safe handling

Handling requirements: Avoid direct contact with the substance. Avoid the formation or spread of mists in the air.
Ensure there is sufficient ventilation of the area. Only use in fume hood.

7.2. Conditions for safe storage, including any incompatibilities

Storage conditions: 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.

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 sufficient ventilation of the area.

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

Hand protection: Protective gloves.

Eye protection: Safety glasses. 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: Colourless

Also soluble in: Hexane. Acetonitrile. Methylene chloride.

Boiling point/range °C: 80-81@54mmHg

Flash point °C: 65

Relative density: 1.414

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.

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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). Sulphur oxides (SOx)

Section 11: Toxicological information

11.1. Information on toxicological effects

Toxicity values:

Route	Species	Test	Value	Units
ORAL	RAT	LD50	50-300	mg/kg

Relevant hazards for substance:

Hazard	Route	Basis
Acute toxicity (ac. tox. 3)	ING	Based on test data
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.

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.

Delayed / immediate effects: Immediate effects can be expected after short-term exposure.

Other information: High hazard Class III chemical : assigned according to Cramer decision tree with extensions (predicted *)

Section 12: Ecological information

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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.

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: UN2810

14.2. UN proper shipping name

Shipping name: TOXIC LIQUID, ORGANIC, N.O.S.
(4-Methylphenylsulphur pentafluoride)

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

[cont...]

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14.6. Special precautions for user

Special precautions: No special precautions.

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: Toxic if swallowed.
H315: Causes skin irritation.
H319: Causes serious eye irritation.
R25: Toxic if swallowed.
R36/38: Irritating to eyes and skin.

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