

## SAFETY DATA SHEET

4-METHYL-3-[(THIEN-3-YL)METHYL]-5-THIO-4H-1,2,4-TRIAZOLE

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Compilation date: 24/04/2007

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Revision No: 2

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

#### 1.1. Product identifier

**Product name:** 4-METHYL-3-[(THIEN-3-YL)METHYL]-5-THIO-4H-1,2,4-TRIAZOLE

**CAS number:** 262610-50-4

**Product code:** OR0143

**Synonyms:** 4-METHYL-5-[(THIEN-3-YL)METHYL]-4H-1,2,4-TRIAZOLE-3-THIOL  
3-[(4-METHYL-5-SULPHANYL-4H-1,2,4-TRIAZOL-3-YL)METHYL]THIOPHENE

#### 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:** -: R10; Xn: R22; Xi: R36/37/38

**Classification under CLP:** STOT SE 3: H335; Acute Tox. 4: H302; Eye Irrit. 2: H319; Flam. Sol. 1: H228; Skin Irrit. 2: H315

**Most important adverse effects:** Flammable. Harmful if swallowed. Irritating to eyes, respiratory system and skin.

#### 2.2. Label elements

**Label elements under CLP:**

**Hazard statements:** H228: Flammable solid.

H302: Harmful if swallowed.

H315: Causes skin irritation.

H319: Causes serious eye irritation.

H335: May cause respiratory irritation.

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**Signal words:** Danger

**Hazard pictograms:** GHS02: Flame

GHS07: Exclamation mark



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

P210: Keep away from heat/sparks/open flames/hot surfaces. - No smoking.

**Label elements under CHIP:**

**Hazard symbols:** Harmful.



**Risk phrases:** R10: Flammable.

R22: Harmful if swallowed.

R36/37/38: Irritating to eyes, respiratory system and skin.

**Safety phrases:** S22: Do not breathe dust.

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:** In use, may form flammable / explosive vapour-air mixture. Stench.

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

## Section 3: Composition/information on ingredients

### 3.1. Substances

**Chemical identity:** 4-METHYL-3-[(THIEN-3-YL)METHYL]-5-THIO-4H-1,2,4-TRIAZOLE

## 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.

[cont...]

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**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:** Flammable. In combustion emits toxic fumes. Forms explosive air-vapour mixture. Carbon oxides. Sulphur oxides (SO<sub>x</sub>).

### 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:** 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. Turn leaking containers leak-side up to prevent the escape of liquid. Eliminate all sources of ignition.

### 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. Do not use equipment in clean-up procedure which may produce sparks.

### 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 mists in the air. Smoking is forbidden. Use non-sparking tools. Only use in fume hood.

[cont...]

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## 7.2. Conditions for safe storage, including any incompatibilities

**Storage conditions:** Store in cool, well ventilated area. Keep container tightly closed. Keep away from sources of ignition. Prevent the build up of electrostatic charge in the immediate area. Ensure lighting and electrical equipment are not a source of ignition. 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:** Not applicable.

### 8.2. Exposure controls

**Engineering measures:** Ensure there is sufficient ventilation of the area. Ensure lighting and electrical equipment are not a source of ignition.

**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:** Powder

**Colour:** White

**Odour:** STENCH

**Melting point/range °C:** 130-133

### 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. Stable at room temperature.

### 10.3. Possibility of hazardous reactions

**Hazardous reactions:** Hazardous reactions will not occur under normal transport or storage conditions.

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### 10.4. Conditions to avoid

**Conditions to avoid:** Heat. Hot surfaces. Sources of ignition. 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. Sulphur oxides (SO<sub>x</sub>)

## Section 11: Toxicological information

### 11.1. Information on toxicological effects

#### Relevant hazards for substance:

Hazard	Route	Basis
Acute toxicity (ac. tox. 4)	ING	Based on test data
Skin corrosion/irritation	DRM	Based on test data
Serious eye damage/irritation	OPT	Based on test data
STOT-single exposure	INH	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 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:** Not applicable.

### 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.

[cont...]

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### 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:** UN1325

### 14.2. UN proper shipping name

**Shipping name:** FLAMMABLE SOLID, ORGANIC, N.O.S.

### 14.3. Transport hazard class(es)

**Transport class:** 4.1

### 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:** 3

## 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.

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\* Data predicted using computational software. Toxtree - Toxic Hazard Estimation by decision tree approach. [http://ecb.jrc.ec.europa.eu/qsar/qsar-tools/index.php?](http://ecb.jrc.ec.europa.eu/qsar/qsar-tools/index.php?c=TOXTREE)

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/](http://www.acdlabs.com/products/pc_admet/tox/tox/)

**Phrases used in s.2 and 3:** H228: Flammable solid.

H302: Harmful if swallowed.

H315: Causes skin irritation.

H319: Causes serious eye irritation.

H335: May cause respiratory irritation.

R10: Flammable.

R22: Harmful if swallowed.

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**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.

