

**SAFETY DATA SHEET**  
(2S)-3-(ACETYLTHIO)-2-METHYLPROPANOIC ACID

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**Compilation date:** 03/07/2012  
**Revision date:** 05/07/2012  
**Revision No:** 2

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

**1.1. Product identifier**

**Product name:** (2S)-3-(ACETYLTHIO)-2-METHYLPROPANOIC ACID  
**CAS number:** 76497-39-7  
**EINECS number:** 278-480-8  
**Product code:** OR61506  
**Synonyms:** (2S)-3-(ACETYSULPHANYL)-2-METHYLPROPANOIC ACID  
(2S)-3-(ACETYLTHIO)-2-METHYLPROPIONIC ACID

**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:** Xn: R22; C: R34  
**Classification under CLP:** Acute Tox. 4: H302; Skin Corr. 1B: H314  
**Most important adverse effects:** Harmful if swallowed. Causes burns.

**2.2. Label elements**

**Label elements under CLP:**

**Hazard statements:** H302: Harmful if swallowed.  
H314: Causes severe skin burns and eye damage.  
**Signal words:** Danger  
**Hazard pictograms:** GHS05: Corrosion  
GHS07: Exclamation mark

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**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:** Corrosive.



**Risk phrases:** R22: Harmful if swallowed.  
R34: Causes burns.

### 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:** (2S)-3-(ACETYLTHIO)-2-METHYLPROPANOIC ACID

## 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.  
Drench the affected skin with running water for 10 minutes or longer if substance is still on skin. Transfer to hospital if there are burns or symptoms of poisoning.
- 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. Give 1 cup of water to drink every 10 minutes. 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. If unconscious and breathing is OK, place in the recovery position. If conscious, ensure the casualty sits or lies down. If breathing becomes bubbly, have the casualty sit and provide oxygen if available. Transfer to hospital as soon as possible.

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

- Skin contact:** Blistering may occur. Progressive ulceration will occur if treatment is not immediate.
- Eye contact:** Corneal burns may occur. May cause permanent damage.
- Ingestion:** Corrosive burns may appear around the lips. Blood may be vomited. There may be bleeding from the mouth or nose.

[cont...]

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**Inhalation:** There may be shortness of breath with a burning sensation in the throat. 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. Use water spray to cool containers.

### 5.2. Special hazards arising from the substance or mixture

**Exposure hazards:** Corrosive. In combustion emits toxic fumes. 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:** 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

## 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. 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.

**Suitable packaging:** Must only be kept in original packaging.

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## 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.

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

**Hand protection:** Impermeable gloves.

**Eye protection:** Tightly fitting safety goggles. Ensure eye bath is to hand.

**Skin protection:** Impermeable protective clothing.

## Section 9: Physical and chemical properties

### 9.1. Information on basic physical and chemical properties

**State:** Liquid

**Colour:** Pale yellow

**Boiling point/range °C:** 131-132@2.25mmHg

**Melting point/range °C:** 5

**Flash point °C:** >112.8

**Relative density:** 1.178

### 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.

### 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. Sulphur oxides (SO<sub>x</sub>)

[cont...]

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## 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

### Symptoms / routes of exposure

**Skin contact:** Blistering may occur. Progressive ulceration will occur if treatment is not immediate.

**Eye contact:** Corneal burns may occur. May cause permanent damage.

**Ingestion:** Corrosive burns may appear around the lips. Blood may be vomited. There may be bleeding from the mouth or nose.

**Inhalation:** There may be shortness of breath with a burning sensation in the throat. 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.

### 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.

[cont...]

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### Section 14: Transport information

#### 14.1. UN number

UN number: UN3265

#### 14.2. UN proper shipping name

Shipping name: CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S.

#### 14.3. Transport hazard class(es)

Transport class: 8

#### 14.4. Packing group

Packing group: II

#### 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

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

**Phrases used in s.2 and 3:** H302: Harmful if swallowed.

H314: Causes severe skin burns and eye damage.

R22: Harmful if swallowed.

R34: Causes burns.

**Legal disclaimer:** The material is intended for research purposes only and should be handled exclusively

[cont...]

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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.