

## SAFETY DATA SHEET

ETHYL 5-ACETYL-3-METHYLISOXAZOLE-4-CARBOXYLATE

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Compilation date: 17/01/2012

Revision No: 1

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

#### 1.1. Product identifier

**Product name:** ETHYL 5-ACETYL-3-METHYLISOXAZOLE-4-CARBOXYLATE  
**CAS number:** 129663-13-4  
**Product code:** OR29731  
**Synonyms:** ETHYL 5-ACETYL-3-METHYL-1,2-OXAZOLE-4-CARBOXYLATE  
5-ACETYL-4-(ETHOXYCARBONYL)-3-METHYLISOXAZOLE  
5-ACETYL-4-(ETHOXYCARBONYL)-3-METHYL-1,2-OXAZOLE

#### 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:** -: R14; Xn: R20/21/22; Xi: R36/37/38

**Classification under CLP:** Acute Tox. 4: H302+312+332; STOT SE 3: H335; Eye Irrit. 2: H319; Skin Irrit. 2: H315

**Most important adverse effects:** Reacts violently with water. Harmful by inhalation, in contact with skin and if swallowed.  
Irritating to eyes, respiratory system and skin.

#### 2.2. Label elements

##### Label elements under CLP:

**Hazard statements:** H302+312+332: Harmful if swallowed, in contact with skin or if inhaled.  
H315: Causes skin irritation.  
H319: Causes serious eye irritation.  
H335: May cause respiratory irritation.

**Signal words:** Warning

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**Hazard pictograms:** GHS07: Exclamation mark



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

**Label elements under CHIP:**

**Hazard symbols:** Harmful.



**Risk phrases:** R14: Reacts violently with water.  
R20/21/22: Harmful by inhalation, in contact with skin and if swallowed.  
R36/37/38: Irritating to eyes, respiratory system and skin.

**Safety phrases:** S36/37/39: Wear suitable protective clothing, gloves and eye / face protection.

## 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:** ETHYL 5-ACETYL-3-METHYLISOXAZOLE-4-CARBOXYLATE

## 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. 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 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. 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 pain and redness. The eyes may water profusely.

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

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

[cont...]

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**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:** Not applicable.

## 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. Do not use water.

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

**Exposure hazards:** In combustion emits toxic fumes of carbon dioxide / carbon monoxide. Nitrogen oxides (NO<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. 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.

### 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. Light Sensitive. Moisture sensitive.

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

[cont...]

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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:** Respiratory protection not required.

**Hand protection:** Impermeable gloves.

**Eye protection:** Safety glasses with side-shields. 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

**Boiling point/range °C:** 95/0.5mmHg

### 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. Reacts violently with water

### 10.4. Conditions to avoid

**Conditions to avoid:** Heat. Light. Moist air.

### 10.5. Incompatible materials

**Materials to avoid:** Strong oxidising agents. Strong acids. Water.

### 10.6. Hazardous decomposition products

**Haz. decomp. products:** In combustion emits toxic fumes of carbon dioxide / carbon monoxide. Nitrogen oxides (NO<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)	INH DRM 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 pain and redness. The eyes may water profusely.

**Ingestion:** There may be soreness and redness of the mouth and throat. There may be difficulty swallowing. 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.

**Other information:** High hazard Class III chemical : assigned according to Cramer decision tree with extensions (predicted \*) No structural alert for carcinogenicity (predicted \*)

## Section 12: Ecological information

### 12.1. Toxicity

**Ecotoxicity values:** Not applicable.

### 12.2. Persistence and degradability

**Persistence and degradability:** Easily biodegradable (predicted \*)

### 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

[cont...]

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**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.

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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?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+312+332: Harmful if swallowed, in contact with skin or if inhaled.

H315: Causes skin irritation.

H319: Causes serious eye irritation.

H335: May cause respiratory irritation.

R14: Reacts violently with water.

R20/21/22: Harmful by inhalation, in contact with skin and if swallowed.

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

**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.