

## SAFETY DATA SHEET

Version 4.5  
Revision Date 05/11/2016  
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1. PRODUCT AND COMPANY IDENTIFICATION

## 1.1 Product identifiers

Product name : 3-Thiopheneacetonitrile

Product Number : 219193  
Brand : Aldrich

CAS-No. : 13781-53-8

## 1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Synthesis of substances

## 1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich  
3050 Spruce Street  
SAINT LOUIS MO 63103  
USA

Telephone : +1 800-325-5832  
Fax : +1 800-325-5052

## 1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

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2. HAZARDS IDENTIFICATION

## 2.1 Classification of the substance or mixture

**GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Acute toxicity, Oral (Category 4), H302  
Acute toxicity, Inhalation (Category 4), H332  
Acute toxicity, Dermal (Category 4), H312  
Skin irritation (Category 2), H315  
Eye irritation (Category 2A), H319  
Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335

For the full text of the H-Statements mentioned in this Section, see Section 16.

## 2.2 GHS Label elements, including precautionary statements

Pictogram



Signal word : Warning

Hazard statement(s)  
H302 + H312 + H332  
H315  
H319  
H335

Harmful if swallowed, in contact with skin or if inhaled  
Causes skin irritation.  
Causes serious eye irritation.  
May cause respiratory irritation.

Precautionary statement(s)  
P261  
P264  
P270

Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.  
Wash skin thoroughly after handling.  
Do not eat, drink or smoke when using this product.

P271	Use only outdoors or in a well-ventilated area.
P280	Wear eye protection/ face protection.
P280	Wear protective gloves/ protective clothing.
P301 + P312 + P330	IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell. Rinse mouth.
P302 + P352	IF ON SKIN: Wash with plenty of soap and water.
P302 + P352 + P312	IF ON SKIN: Wash with plenty of soap and water. Call a POISON CENTER or doctor/ physician if you feel unwell.
P304 + P340 + P312	IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing. Call a POISON CENTER or doctor/ physician if you feel unwell.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P332 + P313	If skin irritation occurs: Get medical advice/ attention.
P337 + P313	If eye irritation persists: Get medical advice/ attention.
P362	Take off contaminated clothing and wash before reuse.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
P405	Store locked up.
P501	Dispose of contents/ container to an approved waste disposal plant.

## 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

## 3. COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1 Substances

Synonyms : 3-Thienylacetonitrile

Formula : C<sub>6</sub>H<sub>5</sub>NS

Molecular weight : 123.18 g/mol

CAS-No. : 13781-53-8

EC-No. : 237-433-1

#### Hazardous components

Component	Classification	Concentration
<b>3-Thienylacetonitrile</b>		
	Acute Tox. 4; Skin Irrit. 2; Eye Irrit. 2A; STOT SE 3; H302 + H312 + H332, H315, H319, H335	<= 100 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

## 4. FIRST AID MEASURES

### 4.1 Description of first aid measures

#### General advice

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

#### If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

#### In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

#### In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

#### If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

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

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

- 4.3 Indication of any immediate medical attention and special treatment needed**  
No data available

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## 5. FIREFIGHTING MEASURES

- 5.1 Extinguishing media**  
**Suitable extinguishing media**  
Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.
- 5.2 Special hazards arising from the substance or mixture**  
No data available
- 5.3 Advice for firefighters**  
Wear self-contained breathing apparatus for firefighting if necessary.
- 5.4 Further information**  
No data available

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## 6. ACCIDENTAL RELEASE MEASURES

- 6.1 Personal precautions, protective equipment and emergency procedures**  
Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas.  
For personal protection see section 8.
- 6.2 Environmental precautions**  
Do not let product enter drains.
- 6.3 Methods and materials for containment and cleaning up**  
Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.
- 6.4 Reference to other sections**  
For disposal see section 13.

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## 7. HANDLING AND STORAGE

- 7.1 Precautions for safe handling**  
Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.  
For precautions see section 2.2.
- 7.2 Conditions for safe storage, including any incompatibilities**  
Keep container tightly closed in a dry and well-ventilated place.  
Storage class (TRGS 510): Non-combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials
- 7.3 Specific end use(s)**  
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

- 8.1 Control parameters**  
**Components with workplace control parameters**  
Contains no substances with occupational exposure limit values.
- 8.2 Exposure controls**  
**Appropriate engineering controls**  
Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.
- Personal protective equipment**  
**Eye/face protection**  
Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

### Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

#### Full contact

Material: butyl-rubber

Minimum layer thickness: 0.3 mm

Break through time: 480 min

Material tested: Butoject® (KCL 897 / Aldrich Z677647, Size M)

#### Splash contact

Material: Nature latex/chloroprene

Minimum layer thickness: 0.6 mm

Break through time: 60 min

Material tested: Lapren® (KCL 706 / Aldrich Z677558, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

### Body Protection

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

### Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

### Control of environmental exposure

Do not let product enter drains.

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## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

- |   |  |
|---|--|
| a) Appearance                                   | Form: clear, liquid<br>Colour: brown                   |
| b) Odour  | No data available                                      |
| c) Odour Threshold                              | No data available                                      |
| d) pH   | No data available                                      |
| e) Melting point/freezing point                 | No data available                                      |
| f) Initial boiling point and boiling range      | 124 - 125 °C (255 - 257 °F) at 21 hPa (16 mmHg) - lit. |
| g) Flash point                                  | 119 °C (246 °F) - closed cup                           |
| h) Evaporation rate                             | No data available                                      |
| i) Flammability (solid, gas)                    | No data available                                      |
| j) Upper/lower flammability or explosive limits | No data available                                      |
| k) Vapour pressure                              | No data available                                      |
| l) Vapour density                               | No data available                                      |
| m) Relative density                             | 1.08 g/cm <sup>3</sup> at 25 °C (77 °F)                |

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|----|--|-------------------|
| n) | Water solubility                       | No data available |
| o) | Partition coefficient: n-octanol/water | No data available |
| p) | Auto-ignition temperature              | No data available |
| q) | Decomposition temperature              | No data available |
| r) | Viscosity                              | No data available |
| s) | Explosive properties                   | No data available |
| t) | Oxidizing properties                   | No data available |

## 9.2 Other safety information

No data available

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## 10. STABILITY AND REACTIVITY

### 10.1 Reactivity

No data available

### 10.2 Chemical stability

Stable under recommended storage conditions.

### 10.3 Possibility of hazardous reactions

No data available

### 10.4 Conditions to avoid

No data available

### 10.5 Incompatible materials

Strong acids, Strong bases, Strong oxidizing agents, Strong reducing agents

### 10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NO<sub>x</sub>), Sulphur oxides, Hydrogen cyanide (hydrocyanic acid)

Other decomposition products - No data available

In the event of fire: see section 5

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## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

No data available

No data available

#### Skin corrosion/irritation

No data available

#### Serious eye damage/eye irritation

No data available

#### Respiratory or skin sensitisation

No data available

#### Germ cell mutagenicity

No data available

#### Carcinogenicity

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

**Reproductive toxicity**

No data available

No data available

**Specific target organ toxicity - single exposure**

Inhalation - May cause respiratory irritation.

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**Additional Information**

RTECS: Not available

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

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## 12. ECOLOGICAL INFORMATION

### 12.1 Toxicity

No data available

### 12.2 Persistence and degradability

No data available

### 12.3 Bioaccumulative potential

No data available

### 12.4 Mobility in soil

No data available

### 12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

### 12.6 Other adverse effects

No data available

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## 13. DISPOSAL CONSIDERATIONS

### 13.1 Waste treatment methods

**Product**

Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

**Contaminated packaging**

Dispose of as unused product.

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## 14. TRANSPORT INFORMATION

**DOT (US)**

UN number: 3276      Class: 6.1      Packing group: II  
Proper shipping name: Nitriles, liquid, toxic, n.o.s. (3-Thienylacetonitrile)  
Reportable Quantity (RQ):

Poison Inhalation Hazard: No

**IMDG**

UN number: 3276      Class: 6.1      Packing group: II      EMS-No: F-A, S-A

Proper shipping name: NITRILES, LIQUID, TOXIC, N.O.S. (3-Thienylacetonitrile)

#### IATA

UN number: 3276

Class: 6.1

Packing group: II

Proper shipping name: Nitriles, liquid, toxic, n.o.s. (3-Thienylacetonitrile)

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### 15. REGULATORY INFORMATION

#### SARA 302 Components

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

#### SARA 313 Components

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

#### SARA 311/312 Hazards

Acute Health Hazard

#### Massachusetts Right To Know Components

No components are subject to the Massachusetts Right to Know Act.

#### Pennsylvania Right To Know Components

	CAS-No.	Revision Date
3-Thienylacetonitrile	13781-53-8	

#### New Jersey Right To Know Components

	CAS-No.	Revision Date
3-Thienylacetonitrile	13781-53-8	

#### California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

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### 16. OTHER INFORMATION

#### Full text of H-Statements referred to under sections 2 and 3.

Acute Tox.	Acute toxicity
Eye Irrit.	Eye irritation
H302	Harmful if swallowed.
H302 + H312 + H332	Harmful if swallowed, in contact with skin or if inhaled
H312	Harmful in contact with skin.
H315	Causes skin irritation.
H319	Causes serious eye irritation.

#### HMIS Rating

Health hazard:	2
Chronic Health Hazard:	
Flammability:	1
Physical Hazard	0

#### NFPA Rating

Health hazard:	2
Fire Hazard:	1
Reactivity Hazard:	0

#### Further information

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or from contact with the above product. See [www.sigma-aldrich.com](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

**Preparation Information**

Sigma-Aldrich Corporation  
Product Safety – Americas Region  
1-800-521-8956

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