

## SAFETY DATA SHEET

Version 5.2  
Revision Date 06/25/2014  
Print Date 02/15/2018

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1. PRODUCT AND COMPANY IDENTIFICATION

## 1.1 Product identifiers

Product name : Acetyl isothiocyanate

Product Number : 01230  
Brand : Sigma

CAS-No. : 13250-46-9

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

Identified uses : Laboratory chemicals, Manufacture 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 3), H301  
Acute toxicity, Inhalation (Category 3), H331  
Acute toxicity, Dermal (Category 3), H311  
Skin irritation (Category 2), H315  
Eye irritation (Category 2A), H319  
Respiratory sensitisation (Category 1), H334  
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

Danger

Hazard statement(s)

H301 + H311 + H331

H315

H319

H334

H335

Toxic if swallowed, in contact with skin or if inhaled

Causes skin irritation.

Causes serious eye irritation.

May cause allergy or asthma symptoms or breathing difficulties if inhaled.

May cause respiratory irritation.

Precautionary statement(s)

P261

P264

Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.

Wash skin thoroughly after handling.

P270	Do not eat, drink or smoke when using this product.
P271	Use only outdoors or in a well-ventilated area.
P280	Wear protective gloves/ eye protection/ face protection.
P285	In case of inadequate ventilation wear respiratory protection.
P301 + P310	IF SWALLOWED: Immediately call a POISON CENTER or doctor/ physician.
P302 + P352	IF ON SKIN: Wash with plenty of soap and water.
P304 + P340	IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P322	Specific measures (see supplemental first aid instructions on this label).
P330	Rinse mouth.
P332 + P313	If skin irritation occurs: Get medical advice/ attention.
P337 + P313	If eye irritation persists: Get medical advice/ attention.
P342 + P311	If experiencing respiratory symptoms: Call a POISON CENTER or doctor/ physician.
P361	Remove/ Take off immediately all contaminated clothing.
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

Reacts violently with water.  
Lachrymator.

## 3. COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1 Substances

Formula :  $C_3H_3NOS$   
Molecular Weight : 101.13 g/mol  
CAS-No. : 13250-46-9

#### Hazardous components

Component	Classification	Concentration
<b>Acetyl isothiocyanate</b>		
	Acute Tox. 3; Skin Irrit. 2; Eye Irrit. 2A; Resp. Sens. 1; STOT SE 3; H301 + H311 + H331, H315, H319, H334, H335	-

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. Take victim immediately to hospital. 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**  
Dry powder

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

Carbon oxides, nitrogen oxides (NO<sub>x</sub>), Sulphur oxides

### **5.3 Advice for firefighters**

Wear self contained breathing apparatus for fire fighting 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**

Wear respiratory protection. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas.

For personal protection see section 8.

### **6.2 Environmental precautions**

Prevent further leakage or spillage if safe to do so. 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. Do not flush with water. 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. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Never allow product to get in contact with water during storage.

Recommended storage temperature: -20 °C

Store under inert gas. Moisture sensitive.

### **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**

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

## 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.

### Body Protection

Complete suit protecting against chemicals, Flame retardant protective clothing, 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

Prevent further leakage or spillage if safe to do so. 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: liquid                             |
| b) Odour  | Stench.                                  |
| 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      | 132 - 133 °C (270 - 271 °F) - lit.       |
| g) Flash point                                  | no data available                        |
| 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                             | 1.151 g/cm <sup>3</sup> at 20 °C (68 °F) |
| 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

Reacts violently with water.

### 10.4 Conditions to avoid

Exposure to moisture.

### 10.5 Incompatible materials

Strong oxidizing agents

### 10.6 Hazardous decomposition products

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

#### 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

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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. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

**Contaminated packaging**

Dispose of as unused product.

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**14. TRANSPORT INFORMATION****DOT (US)**

UN number: 2810      Class: 6.1      Packing group: II  
Proper shipping name: Toxic, liquids, organic, n.o.s. (Acetyl isothiocyanate)  
Marine pollutant: No  
Poison Inhalation Hazard: No

**IMDG**

UN number: 2810      Class: 6.1      Packing group: II      EMS-No: F-A, S-A  
Proper shipping name: TOXIC LIQUID, ORGANIC, N.O.S. (Acetyl isothiocyanate)  
Marine pollutant: No

**IATA**

UN number: 2810      Class: 6.1      Packing group: II  
Proper shipping name: Toxic liquid, organic, n.o.s. (Acetyl isothiocyanate)

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**15. REGULATORY INFORMATION****SARA 302 Components**

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

**SARA 313 Components**

SARA 313: 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**

Acetyl isothiocyanate

CAS-No.  
13250-46-9

Revision Date

**New Jersey Right To Know Components**

Acetyl isothiocyanate

CAS-No.  
13250-46-9

Revision Date

**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
H301	Toxic if swallowed.
H301 + H311 + H331	Toxic if swallowed, in contact with skin or if inhaled
H311	Toxic in contact with skin.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H331	Toxic if inhaled.
H334	May cause allergy or asthma symptoms or breathing difficulties if inhaled.

**HMIS Rating**

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

**NFPA Rating**

Health hazard:	2
Fire Hazard:	0
Reactivity Hazard:	2
Health hazard:	4
Fire Hazard:	0
Reactivity Hazard:	0

**Further information**

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The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling 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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