

## SAFETY DATA SHEET

Version 6.7  
Revision Date 01/21/2021  
Print Date 02/05/2022

**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : *N*-Allylthiourea

Product Number : 108804  
Brand : Aldrich  
CAS-No. : 109-57-9

**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 Inc.  
3050 SPRUCE ST  
ST. LOUIS MO 63103  
UNITED STATES

Telephone : +1 314 771-5765  
Fax : +1 800 325-5052

**1.4 Emergency telephone**

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-  
527-3887 CHEMTREC (International) 24  
Hours/day; 7 Days/week

**SECTION 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

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 : Toxic if swallowed.

Precautionary statement(s)  
P264 : Wash skin thoroughly after handling.

Aldrich - 108804

Page 1 of 7

P270	Do not eat, drink or smoke when using this product.
P301 + P310 + P330	IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth.
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

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Synonyms : Thiosinamine  
1-Allyl-2-thiourea

Formula :  $C_4H_8N_2S$   
Molecular weight : 116.18 g/mol  
CAS-No. : 109-57-9  
EC-No. : 203-683-5

Component	Classification	Concentration
<b>N-Allylthiourea</b>		
	Acute Tox. 3; H301	<= 100 %

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

## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

No data available

### 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

## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

No data available

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

Carbon oxides  
Nitrogen oxides (NO<sub>x</sub>)  
Sulfur oxides  
Combustible.

### 5.3 Advice for firefighters

No data available

## 5.4 Further information

No data available

---

## SECTION 6: Accidental release measures

### 6.1 Personal precautions, protective equipment and emergency procedures

For personal protection see section 8.

### 6.2 Environmental precautions

No data available

### 6.3 Methods and materials for containment and cleaning up

No data available

### 6.4 Reference to other sections

For disposal see section 13.

---

## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

For precautions see section 2.2.

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

No data available

### 7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

---

## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

### 8.2 Exposure controls

#### Personal protective equipment

##### Skin protection

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: KCL 741 Dermatril® L

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please

contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: KCL 741 Dermatril® L

### **Control of environmental exposure**

Prevent product from entering drains.

---

## **SECTION 9: Physical and chemical properties**

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

a) Appearance	Form: crystalline Color: beige
b) Odor	unpleasant
c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/range: 70 - 72 °C (158 - 162 °F) - lit.
f) Initial boiling point and boiling range	No data available
g) Flash point	( )Not applicable
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	No data available
k) Vapor pressure	No data available
l) Vapor density	No data available
m) Relative density	1.11 g/mL at 25 °C (77 °F)
n) Water solubility	No data available
o) Partition coefficient: n-octanol/water	No data available
p) Autoignition 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

Aldrich - 108804

Page 4 of 7

---

## SECTION 10: Stability and reactivity

### 10.1 Reactivity

No data available

### 10.2 Chemical stability

No data available

### 10.3 Possibility of hazardous reactions

Violent reactions possible with:  
Strong oxidizing agents

### 10.4 Conditions to avoid

No data available

### 10.5 Incompatible materials

no information available

### 10.6 Hazardous decomposition products

In the event of fire: see section 5

---

## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - 200 mg/kg

Remarks:

(RTECS)

Inhalation: No data available

Dermal: No data available

No data available

#### Skin corrosion/irritation

No data available

#### Serious eye damage/eye irritation

No data available

#### Respiratory or skin sensitization

No data available

#### Germ cell mutagenicity

No data available

#### Carcinogenicity

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

NTP: No ingredient 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 on OSHA's list of regulated carcinogens.

**Reproductive toxicity**

No data available

**Specific target organ toxicity - single exposure**

No data available

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**11.2 Additional Information**

RTECS: YR8050000

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

---

**SECTION 12: Ecological information****12.1 Toxicity**

Toxicity to fish                      LC50 - *Leuciscus idus melanotus* - 3,200 mg/l - 48 h

Toxicity to daphnia                      LC50 - *Daphnia magna* (Water flea) - 39 mg/l - 24 h  
and other aquatic  
invertebrates

**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

---

**SECTION 13: Disposal considerations****13.1 Waste treatment methods**

No data available

---

**SECTION 14: Transport information****DOT (US)**

UN number: 2811    Class: 6.1

Packing group: III

Proper shipping name: Toxic solids, organic, n.o.s. (N-Allylthiourea)

Aldrich - 108804

Page 6 of 7

Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

**IMDG**

UN number: 2811    Class: 6.1    Packing group: III    EMS-No: F-A, S-A  
Proper shipping name: TOXIC SOLID, ORGANIC, N.O.S. (N-Allylthiourea)

**IATA**

UN number: 2811    Class: 6.1    Packing group: III  
Proper shipping name: Toxic solid, organic, n.o.s. (N-Allylthiourea)

---

**SECTION 15: Regulatory information****SARA 302 Components**

This material does not contain any components with a section 302 EHS TPQ.

**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.

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

**Pennsylvania Right To Know Components**

N-Allylthiourea	CAS-No. 109-57-9	Revision Date
-----------------	---------------------	---------------

**New Jersey Right To Know Components**

N-Allylthiourea	CAS-No. 109-57-9	Revision Date
-----------------	---------------------	---------------

---

**SECTION 16: Other information**

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact [mlsbranding@sial.com](mailto:mlsbranding@sial.com).

Version: 6.7    Revision Date: 01/21/2021    Print Date: 02/05/2022