

## SAFETY DATA SHEET

Version 6.0  
Revision Date 11/07/2017  
Print Date 11/16/2018

---

1. PRODUCT AND COMPANY IDENTIFICATION

## 1.1 Product identifiers

Product name : 4-Nitrophenyl isothiocyanate

Product Number : 283541

Brand : Aldrich

CAS-No. : 2131-61-5

## 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 Street  
ST. LOUIS MO 63103  
UNITED STATES

Telephone : +1 314 771-5765

Fax : +1 800 325-5052

## 1.4 Emergency telephone number

Emergency Phone # : (314) 776-6555

---

2. HAZARDS IDENTIFICATION

## 2.1 Classification of the substance or mixture

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

Skin irritation (Category 2), H315

Eye irritation (Category 2A), H319

Respiratory sensitisation (Category 1), H334

Skin sensitisation (Category 1), H317

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 { error: file not found: C:\WWI\graphics\CUST-N15.00931430 } { error: file not found: C:\WWI\graphics\CUST-N15.00931410 }

Signal word CUST-N15.00700525

Hazard statement(s)

H315 Causes skin irritation.

H317 May cause an allergic skin reaction.

H319 Causes serious eye irritation.

H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled.

H335 May cause respiratory irritation.

Precautionary statement(s)	
P261	Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
P264	Wash skin thoroughly after handling.
P271	Use only outdoors or in a well-ventilated area.
P272	Contaminated work clothing should not be allowed out of the workplace.
P280	Wear eye protection/ face protection.
P280	Wear protective gloves.
P285	In case of inadequate ventilation wear respiratory protection.
P302 + P352	IF ON SKIN: Wash with plenty of soap and water.
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.
P333 + P313	If skin irritation or rash 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/doctor.
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

Lachrymator.

## 3. COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1 Substances

Formula	: $C_7H_4N_2O_2S$
Molecular weight	: 180.18 g/mol
CAS-No.	: 2131-61-5
EC-No.	: 218-359-9

#### Hazardous components

Component	Classification	Concentration
<b>4-Nitrobenzyl-isothiocyanate</b>		
	Skin Irrit. 2; Eye Irrit. 2A; Resp. Sens. 1; Skin Sens. 1; STOT SE 3; H315, H317, H319, H334, 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

---

### **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**

Carbon oxides, Nitrogen oxides (NOx), Sulphur oxides

#### **5.3 Advice for firefighters**

Wear self-contained breathing apparatus for firefighting if necessary.

#### **5.4 Further information**

No data available

---

### **6. ACCIDENTAL RELEASE MEASURES**

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

Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust.

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**

Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

#### **6.4 Reference to other sections**

For disposal see section 13.

---

### **7. HANDLING AND STORAGE**

#### **7.1 Precautions for safe handling**

Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Further processing of solid materials may result in the formation of combustible dusts. The potential for combustible dust formation should be taken into consideration before additional processing occurs.

Provide appropriate exhaust ventilation at places where dust is formed.

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.

Moisture sensitive.

Storage class (TRGS 510): 13: Non Combustible Solids

#### **7.3 Specific end use(s)**

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

---

### **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.

### 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

For nuisance exposures use type P95 (US) or type P1 (EU EN 143) particle respirator. For higher level protection use type OV/AG/P99 (US) or type ABEK-P2 (EU EN 143) respirator cartridges. 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.

---

## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

a) Appearance	Form: crystalline Colour: yellow
b) Odour	No data available
c) Odour Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/range: 110 - 112 °C (230 - 234 °F) - lit.
f) Initial boiling point and boiling range	137 - 138 °C (279 - 280 °F) at 15 hPa - 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	No data available
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

---

## 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 oxidizing agents, Strong bases

### 10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NOx), Sulphur oxides

Other decomposition products - No data available

In the event of fire: see section 5

---

## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

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 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

Cough, Shortness of breath, Headache, Nausea, Vomiting, To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

---

**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(4-Nitrobenzyl-isothiocyanate)

**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

---

**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.

---

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

Not dangerous goods

**IMDG**

Not dangerous goods

**IATA**

UN number: 3335

Class: 9

Packing group: III

Proper shipping name: Aviation regulated solid, n.o.s. (4-Nitrobenzyl-isothiocyanate)

---

**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
4-Nitrobenzyl-isothiocyanate	2131-61-5	

**New Jersey Right To Know Components**

	CAS-No.	Revision Date
4-Nitrobenzyl-isothiocyanate	2131-61-5	

**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.

---

**16. OTHER INFORMATION****Full text of H-Statements referred to under sections 2 and 3.**

H315	Causes skin irritation.
H317	May cause an allergic skin reaction.
H319	Causes serious eye irritation.
H334	May cause allergy or asthma symptoms or breathing difficulties if inhaled.
H335	May cause respiratory irritation.

**HMIS Rating**

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

**NFPA Rating**

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

**Further information**

Copyright 2016 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only. 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  
Version: 6.0

Revision Date: 11/07/2017

Print Date: 11/16/2018