

## SAFETY DATA SHEET

Version 6.2  
Revision Date 10/01/2021  
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**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : 2-Nitro-4-thiocyanatoaniline

Product Number : 550647  
Brand : Aldrich  
CAS-No. : 54029-45-7

**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)**

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)  
H315 : Causes skin irritation.

|                            |                                                                                                                                  |
|----------------------------|----------------------------------------------------------------------------------------------------------------------------------|
| H319                       | Causes serious eye irritation.                                                                                                   |
| H335                       | May cause respiratory irritation.                                                                                                |
| Precautionary statement(s) |                                                                                                                                  |
| P261                       | Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.                                                                            |
| P264                       | Wash skin thoroughly after handling.                                                                                             |
| P271                       | Use only outdoors or in a well-ventilated area.                                                                                  |
| P280                       | Wear protective gloves/ eye protection/ face protection.                                                                         |
| P302 + P352                | IF ON SKIN: Wash with plenty of soap and water.                                                                                  |
| P304 + P340 + P312         | IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor 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

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

|                  |                                                                 |
|------------------|-----------------------------------------------------------------|
| Formula          | : C <sub>7</sub> H <sub>5</sub> N <sub>3</sub> O <sub>2</sub> S |
| Molecular weight | : 195.20 g/mol                                                  |
| CAS-No.          | : 54029-45-7                                                    |
| EC-No.           | : 258-931-5                                                     |

| Component                           | Classification                                            | Concentration |
|-------------------------------------|-----------------------------------------------------------|---------------|
| <b>2-Nitro-4-thiocyanatoaniline</b> |                                                           |               |
|                                     | Skin Irrit. 2; Eye Irrit. 2A; STOT SE 3; H315, H319, H335 | <= 100 %      |
| <b>ammonium chloride</b>            |                                                           |               |
|                                     | Acute Tox. 4; Eye Irrit. 2A; H302, H319                   | >= 5 - < 10 % |

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

#### General advice

Show this material safety data sheet to the doctor in attendance.

**If inhaled**

After inhalation: fresh air.

**In case of skin contact**

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.

**In case of eye contact**

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

**If swallowed**

After swallowing: immediately make victim drink water (two glasses at most). 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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**SECTION 5: Firefighting measures****5.1 Extinguishing media****Suitable extinguishing media**

Water Foam Carbon dioxide (CO<sub>2</sub>) Dry powder

**Unsuitable extinguishing media**

For this substance/mixture no limitations of extinguishing agents are given.

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

Carbon oxides

Nitrogen oxides (NO<sub>x</sub>)

Sulfur oxides

Hydrogen chloride gas

Mixture with combustible ingredients.

Development of hazardous combustion gases or vapours possible in the event of fire.

**5.3 Advice for firefighters**

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

**5.4 Further information**

Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

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**SECTION 6: Accidental release measures****6.1 Personal precautions, protective equipment and emergency procedures**

Advice for non-emergency personnel: Avoid inhalation of dusts. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

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**

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

## **6.4 Reference to other sections**

For disposal see section 13.

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## **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**

#### **Storage conditions**

Tightly closed. Dry.

Moisture sensitive. Store under nitrogen.

#### **Storage class**

Storage class (TRGS 510): 11: Combustible Solids

### **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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## **SECTION 8: Exposure controls/personal protection**

### **8.1 Control parameters**

#### **Ingredients with workplace control parameters**

| Component         | CAS-No.    | Value | Control parameters | Basis                                                                                   |
|-------------------|------------|-------|--------------------|-----------------------------------------------------------------------------------------|
| ammonium chloride | 12125-02-9 | TWA   | 10 mg/m3           | USA. ACGIH Threshold Limit Values (TLV)                                                 |
|                   |            | STEL  | 20 mg/m3           | USA. ACGIH Threshold Limit Values (TLV)                                                 |
|                   |            | TWA   | 10 mg/m3           | USA. NIOSH Recommended Exposure Limits                                                  |
|                   |            | ST    | 20 mg/m3           | USA. NIOSH Recommended Exposure Limits                                                  |
|                   |            | PEL   | 10 mg/m3           | California permissible exposure limits for chemical contaminants (Title 8, Article 107) |
|                   |            | STEL  | 20 mg/m3           | California permissible exposure limits for chemical contaminants (Title 8, Article 107) |

## 8.2 Exposure controls

### Appropriate engineering controls

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

### Personal protective equipment

#### Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

#### Skin protection

Handle with impervious gloves.

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

#### Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: KCL 741 Dermatril® L

#### Body Protection

protective clothing

#### Respiratory protection

required when dusts are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

### **Control of environmental exposure**

Do not let product enter drains.

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

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

|                                                 |                                             |
|-------------------------------------------------|---------------------------------------------|
| a) Appearance                                   | Form: solid                                 |
| b) Odor                                         | No data available                           |
| c) Odor Threshold                               | No data available                           |
| d) pH                                           | No data available                           |
| e) Melting point/freezing point                 | Melting point/range: 113 °C (235 °F) - lit. |
| f) Initial boiling point and boiling range      | No data available                           |
| 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) Vapor pressure                               | No data available                           |
| l) Vapor density                                | No data available                           |
| m) Density                                      | No data available                           |
| Relative density                                | No data available                           |
| 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                         | none                                        |

### **9.2 Other safety information**

No data available

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

### 10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

### 10.3 Possibility of hazardous reactions

No data available

### 10.4 Conditions to avoid

no information available

### 10.5 Incompatible materials

Strong oxidizing agents

### 10.6 Hazardous decomposition products

In the event of fire: see section 5

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## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

Acute toxicity estimate Oral - > 5,000 mg/kg  
(Calculation method)

Inhalation: No data available

Acute toxicity estimate Dermal - > 5,000 mg/kg  
(Calculation method)

#### 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**

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

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

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself. See [www.retrologistik.com](http://www.retrologistik.com) for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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

Not dangerous goods

**IMDG**

Not dangerous goods

**IATA**

Not dangerous goods



**Further information**

Not classified as dangerous in the meaning of transport regulations.

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

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

**SARA 313 Components**

The following components are subject to reporting levels established by SARA Title III, Section 313:

|                   | CAS-No.    | Revision Date |
|-------------------|------------|---------------|
| ammonium chloride | 12125-02-9 | 1994-04-01    |

**SARA 311/312 Hazards**

Acute Health Hazard

**Massachusetts Right To Know Components**

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

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**SECTION 16: Other information****Further information**

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.

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