

**SAFETY DATA SHEET**

according to Regulation (EC) No. 1907/2006

Version 6.4

Revision Date 01.04.2023

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GENERIC EU MSDS - NO COUNTRY SPECIFIC DATA - NO OEL DATA

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

Product name : 4-NITROBENZYL THIOCYANATE

Product Number : S432059

Brand : Aldrich

REACH No. : A registration number is not available for this substance as the substance or its uses are exempted from registration, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

CAS-No. : 13287-49-5

**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 (Shanghai) Trading Co.Ltd.  
509 Renqing Road  
Zhangjiang High Tech East Park, Pudong  
SHANGHAI  
201201 SHANGHAI  
CHINA

Telephone : +86 21 6141-5566

Fax : +86 21 6141-5567

**1.4 Emergency telephone**

Emergency Phone # : +86 532 83889090

**SECTION 2: Hazards identification****2.1 Classification of the substance or mixture****Classification according to Regulation (EC) No 1272/2008**

Acute toxicity, Oral (Category 4), H302

Skin sensitization (Category 1), H317

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



## 2.2 Label elements

### Labelling according Regulation (EC) No 1272/2008

Pictogram



Signal Word

Warning

Hazard statement(s)

H302

Harmful if swallowed.

H317

May cause an allergic skin reaction.

Precautionary statement(s)

P280

Wear protective gloves.

Supplemental Hazard Statements

none

## 2.3 Other hazards

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

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## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Formula : C<sub>8</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub>S  
Molecular weight : 194,21 g/mol  
CAS-No. : 13287-49-5

Component	Classification	Concentration
<b>4-NITROBENZYL THIOCYANATE</b>		
CAS-No. 13287-49-5	Acute Tox. 4; Skin Sens. 1; H302, H317	<= 100 %

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

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## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

#### General advice

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

#### 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

Flush eyes with water as a precaution.



**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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**SECTION 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 (NO<sub>x</sub>)

Sulfur oxides

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

Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. 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.

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**SECTION 7: Handling and storage****7.1 Precautions for safe handling****Advice on safe handling**

Avoid contact with skin and eyes. Avoid formation of dust and aerosols.

**Advice on protection against fire and explosion**

Provide appropriate exhaust ventilation at places where dust is formed. Normal measures for preventive fire protection.

### **Hygiene measures**

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

For precautions see section 2.2.

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

### **Storage conditions**

Store in cool place. Keep container tightly closed in a dry and well-ventilated place.

### **Storage class**

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

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

### **8.1 Control parameters**

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

### **8.2 Exposure controls**

#### **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.

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

##### **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.



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## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

- |   |  |
|---|--|
| a) Physical state                               | solid  |
| b) Color  | No data available  |
| c) Odor   | No data available  |
| d) Melting point/freezing point                 | No data available  |
| e) Initial boiling point and boiling range      | No data available  |
| f) Flammability (solid, gas)                    | No data available  |
| g) Upper/lower flammability or explosive limits | No data available  |
| h) Flash point                                  | No data available  |
| i) Autoignition temperature                     | No data available  |
| j) Decomposition temperature                    | No data available  |
| k) pH   | No data available  |
| l) Viscosity                                    | Viscosity, kinematic: No data available<br>Viscosity, dynamic: No data available |
| m) Water solubility                             | No data available  |
| n) Partition coefficient: n-octanol/water       | log Pow: 1,148   |
| o) Vapor pressure                               | No data available  |
| p) Density                                      | No data available  |
| Relative density                                | No data available  |
| q) Relative vapor density                       | No data available  |
| r) Particle characteristics                     | 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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## SECTION 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 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

LD50 Oral - 500,01 mg/kg

Remarks: No data available

Inhalation: No data available

Dermal: No data available

#### Skin corrosion/irritation

Remarks: No data available

#### Serious eye damage/eye irritation

No data available

#### Respiratory or skin sensitization

The preceding data, or interpretation of data, was determined using Quantitative Structure Activity Relationship (QSAR) modeling.

#### Germ cell mutagenicity

No data available

#### Carcinogenicity

No data available

#### 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

### Endocrine disrupting properties

#### Product:

Assessment

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

RTECS: XL1615000

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

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

### 12.6 Endocrine disrupting properties

#### Product:

Assessment

: The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

### 12.7 Other adverse effects

No data available

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## SECTION 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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**SECTION 14: Transport information**

**14.1 UN number**

ADR/RID: -    IMDG: -    IATA: -

**14.2 UN proper shipping name**

ADR/RID: Not dangerous goods

IMDG: Not dangerous goods

IATA: Not dangerous goods

**14.3 Transport hazard class(es)**

ADR/RID: -    IMDG: -    IATA: -

**14.4 Packaging group**

ADR/RID: -    IMDG: -    IATA: -

**14.5 Environmental hazards**

ADR/RID: no    IMDG Marine pollutant: no                          IATA: no

**14.6 Special precautions for user**

No data available

**Further information**

Not classified as dangerous in the meaning of transport regulations.

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**SECTION 15: Regulatory information**

**15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture**

This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.

International Chemical Weapons Convention                          :  
(CWC) Schedules of Toxic Chemicals and  
Precursors

Restrictions on the marketing and use of certain                          :  
dangerous substances and preparations

Regulation (EC) No 649/2012 of the European                          :  
Parliament and the Council concerning the  
export and import of dangerous chemicals

Candidate List of Substances of Very High                          :  
Concern for Authorisation

**15.2 Chemical Safety Assessment**

For this product a chemical safety assessment was not carried out





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## SECTION 16: Other information

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

H302	Harmful if swallowed.
H317	May cause an allergic skin reaction.

### Full text of other abbreviations

ADN - European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways; ADR - Agreement concerning the International Carriage of Dangerous Goods by Road; AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; GHS - Globally Harmonized System; GLP - Good Laboratory Practice; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; n.o.s. - Not Otherwise Specified; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NZIoC - New Zealand Inventory of Chemicals; OECD - Organization for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RID - Regulations concerning the International Carriage of Dangerous Goods by Rail; SADT - Self-Accelerating Decomposition Temperature; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

### Further information

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