# SAFETY DATA SHEET

Version 8.5
Revision Date 09/07/2024
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## SECTION 1: Identification of the substance/mixture and of the company/undertaking

### 1.1 Product identifiers

Product name : Isopropyl isothiocyanate

Product Number : 476013
Brand : Aldrich
CAS-No. : 2253-73-8

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

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

### 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)**

Flammable liquids (Category 3), H226
Skin irritation (Category 2), H315
Eye irritation (Category 2A), H319
Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335



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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 Statements

| | |
|---|---|
| H226 | Flammable liquid and vapor. |
| H315 | Causes skin irritation. |
| H319 | Causes serious eye irritation. |
| H335 | May cause respiratory irritation. |

Precautionary Statements

| | |
|---|---|
| P210 | Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking. |
| P233 | Keep container tightly closed. |
| P240 | Ground/bond container and receiving equipment. |
| P241 | Use explosion-proof electrical/ ventilating/ lighting/ equipment. |
| P242 | Use only non-sparking tools. |
| P243 | Take precautionary measures against static discharge. |
| 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. |
| P303 + P361 + P353 | IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower. |
| 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. |
| P370 + P378 | In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish. |
| P403 + P233 | Store in a well-ventilated place. Keep container tightly closed. |
| P403 + P235 | Store in a well-ventilated place. Keep cool. |
| 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 : Isopropyl mustard oil

Formula : $C_4H_7NS$



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| | | |
|---|---|---|
| Molecular weight | : | 101.17 g/mol |
| CAS-No. | : | 2253-73-8 |
| EC-No. | : | 218-851-3 |

| Component | Classification | Concentration |
|---|---|---|
| **Isopropyl isothiocyanate** | | |
| | Flam. Liq. 3; Skin Irrit. 2; Eye Irrit. 2A; STOT SE 3; H226, H315, H319, H335 | <= 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

**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

## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

**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 (NOx)
Sulfur oxides
Vapors are heavier than air and may spread along floors.



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Forms explosive mixtures with air at elevated temperatures.

### 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

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

## SECTION 6: Accidental release measures

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

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition.
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. Risk of explosion.

### 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 with liquid-absorbent material (e.g. Chemizorb® ). Dispose of properly. Clean up affected area.

### 6.4 Reference to other sections

For disposal see section 13.

## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

**Advice on protection against fire and explosion**

Keep away from open flames, hot surfaces and sources of ignition.Take precautionary measures against static discharge.

**Hygiene measures**

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.
For precautions see section 2.2.

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

**Storage conditions**

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.

**Storage class**

Storage class (TRGS 510): 3: Flammable liquids

### 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**
Contains no substances with occupational exposure limit values.

### 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**
required

**Body Protection**
Flame retardant antistatic protective clothing.

**Respiratory protection**
Recommended Filter type: Filter type ABEK
The entrepeneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.
required when vapours/aerosols 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. Risk of explosion.

## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

| | | |
|---|---|---|
| a) | Appearance | Form: liquid<br>Color: colorless |
| b) | Odor | No data available |
| c) | Odor Threshold | No data available |
| d) | pH | No data available |
| e) | Melting point/freezing point | No data available |



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| | | |
|---|---|---|
| f) | Initial boiling point and boiling range | 29 - 30 °C 84 - 86 °F at 13 hPa - lit. |
| g) | Flash point | 40 °C (104 °F) - closed cup |
| 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 | 0.948 g/cm3 at 25 °C (77 °F) - lit. |
| | 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 | No data available |

**9.2 Other safety information**
No data available

## SECTION 10: Stability and reactivity

**10.1 Reactivity**
Vapor/air-mixtures are explosive at intense warming.

**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**
Heating.

**10.5 Incompatible materials**
Strong bases



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### 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**
Oral: No data available
Inhalation: No data available
Dermal: No data available

**Skin corrosion/irritation**
Remarks: No data available

**Serious eye damage/eye irritation**
Remarks: 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**
Inhalation - May cause respiratory irritation.

**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.

## SECTION 12: Ecological information

### 12.1 Toxicity

No data available



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### 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 Endocrine disrupting properties
No data available

### 12.7 Other adverse effects
No data available

## 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.

## SECTION 14: Transport information

**DOT (US)**
UN number: 1993 Class: 3 Packing group: III
Proper shipping name: Flammable liquids, n.o.s. (Isopropyl isothiocyanate) (Isopropyl isothiocyanate)
Reportable Quantity (RQ):
Poison Inhalation Hazard: No

**IMDG**
UN number: 1993 Class: 3 Packing group: III EMS-No: F-E, S-E
Proper shipping name: FLAMMABLE LIQUID, N.O.S. (Isopropyl isothiocyanate) (Isopropyl isothiocyanate)

**IATA**
UN number: 1993 Class: 3 Packing group: III
Proper shipping name: Flammable liquid, n.o.s. (Isopropyl isothiocyanate) (Isopropyl isothiocyanate)



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## SECTION 15: Regulatory information

### CERCLA Reportable Quantity

This material does not contain any components with a CERCLA RQ.

### SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

### SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

| Components | CAS-No. | Component TPQ (lbs) |
|---|---|---|

**SARA 311/312 Hazards** : Fire Hazard
Acute Health Hazard

**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.

### US State Regulations

### Massachusetts Right To Know

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

### Massachusetts Right To Know

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

### Pennsylvania Right To Know

Isopropyl isothiocyanate 2253-73-8

### Maine Chemicals of High Concern

Product does not contain any listed chemicals

### Vermont Chemicals of High Concern

Product does not contain any listed chemicals

### Washington Chemicals of High Concern

Product does not contain any listed chemicals

### New Jersey Right To Know

Isopropyl isothiocyanate 2253-73-8

### The ingredients of this product are reported in the following inventories:

TSCA : Product contains substance(s) not listed on TSCA inventory.

### TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.



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## SECTION 16: Other information

### Further information

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. 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 and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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