

## Chemical Safety Data Sheet MSDS / SDS

**2-IODOPHENYL ISOTHIOCYANATE**Revision Date:2026-05-31 Revision Number:1

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

Product name : 2-IODOPHENYL ISOTHIOCYANATE  
CBnumber : CB8105691  
CAS : 98041-44-2  
EINECS Number : 622-291-9  
Synonyms : 1-iodo-2-isothiocyanatobenzene,2-Iodophenyl isothiocyanate

**Relevant identified uses of the substance or mixture and uses advised against**

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.  
Uses advised against : none

**Company Identification**

Company : Chemicalbook  
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing  
Telephone : 010-86108875

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**SECTION 2: Hazards identification****GHS Label elements, including precautionary statements**

Symbol(GHS)



Signal word

Danger

**Precautionary statements**

P301+P312 IF SWALLOWED: call a POISON CENTER or doctor/physician IF you feel unwell.

**Hazard statements**

H331 Toxic if inhaled

H314 Causes severe skin burns and eye damage

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**SECTION 3: Composition/information on ingredients****Substance**

Product name : 2-IODOPHENYL ISOTHIOCYANATE

Synonyms	: 1-iodo-2-isothiocyanatobenzene,2-Iodophenyl isothiocyanate
CAS	: 98041-44-2
EC number	: 622-291-9
MF	: C7H4INS
MW	: 261.08

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## SECTION 4: First aid measures

### General Advice

Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.

### Eye Contact

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Immediate medical attention is required.

Keep eye wide open while rinsing.

### Skin Contact

Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes. Call a physician immediately.

### Inhalation

Remove to fresh air. If not breathing, give artificial respiration. Call a physician or poison control center immediately. Do not use mouth-to-mouth method if victim ingested or inhaled the substance; give artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device.

### Ingestion

Immediate medical attention is required. Do NOT induce vomiting. Drink plenty of water. Never give anything by mouth to an unconscious person.

### Most important symptoms and effects

Causes burns by all exposure routes. Product is a corrosive material. Use of gastric lavage or emesis is contraindicated. Possible perforation of stomach or esophagus should be investigated: Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation

### Self-Protection of the First Aider

Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.

### Notes to Physician

Treat symptomatically.

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## SECTION 5: Firefighting measures

### Suitable Extinguishing Media

CO<sub>2</sub>, dry chemical, dry sand, alcohol-resistant foam.

## Extinguishing media which must not be used for safety reasons

No information available.

## Specific Hazards Arising from the Chemical

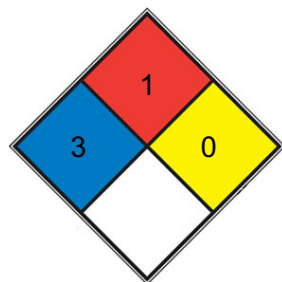
The product causes burns of eyes, skin and mucous membranes.

## Protective Equipment and Precautions for Firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

Thermal decomposition can lead to release of irritating gases and vapors.

## NFPA 704



HEALTH 3 Short exposure could cause serious temporary or moderate residual injury (e.g. [liquid hydrogen](#), [sulfuric acid](#), [calcium hypochlorite](#), hexafluorosilicic acid)

FIRE 1 Materials that require considerable preheating, under all ambient temperature conditions, before ignition and combustion can occur. Includes some finely divided suspended solids that do not require heating before ignition can occur. Flash point at or above 93.3 °C (200 °F). (e.g. [mineral oil](#), ammonia)

REACT 0 Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, [N<sub>2</sub>](#))

SPEC.

HAZ.

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## SECTION 6: Accidental release measures

### Personal Precautions

Use personal protective equipment as required. Evacuate personnel to safe areas. Avoid contact with skin, eyes or clothing.

### Environmental Precautions

Should not be released into the environment. Do not allow material to contaminate ground water system. See Section 12 for additional Ecological Information.

### Methods for Containment and Clean Up

Sweep up and shovel into suitable containers for disposal. Avoid dust formation.

Refer to protective measures listed in Sections 8 and 13.

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## SECTION 7: Handling and storage

## Handling

Wear personal protective equipment/face protection. Do not get in eyes, on skin, or on clothing. Use only under a chemical fume hood. Do not breathe dust. Do not ingest. If swallowed then seek immediate medical assistance.

## Storage

Corrosives area. Keep containers tightly closed in a dry, cool and well-ventilated place.

## Specific Use(s)

Use in laboratories

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## SECTION 8: Exposure controls/personal protection

### Control Parameters

### Monitoring methods

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents. MDHS14/3 General methods for sampling and gravimetric analysis of respirable and inhalable dust

### Exposure Controls

### Engineering Measures

Ensure that eyewash stations and safety showers are close to the workstation location. Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source.

### Personal protective equipment

#### Eye Protection

Goggles (European standard - EN 166)

#### Hand Protection

Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Nitrile rubber	See manufacturers recommendations	-	EN 374	(minimum requirement)
Neoprene				
Natural rubber				
PVC				

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves.

(Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g.

sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

### **Skin and body protection**

Long sleeved clothing

### **Respiratory Protection**

When workers are facing concentrations above the exposure limit they must use appropriate certified respirators.

To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

### **Large scale/emergency use**

Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced

Recommended Filter type: Particulates filter conforming to EN 143

### **Small scale/Laboratory use**

Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

Recommended half mask:- Particle filtering: EN149:2001

When RPE is used a face piece Fit Test should be conducted

### **Hygiene Measures**

Handle in accordance with good industrial hygiene and safety practice.

### **Environmental exposure controls**

No information available.

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## SECTION 9: Physical and chemical properties

### **Information on basic physicochemical properties**

No information available

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### **Physical State**

Solid Crystalline

### **Odor**

No information available

### **Odor Threshold**

No data available

### **pH**

No information available

### **Melting Point/Range**

36 - 39 °C / 96.8 - 102.2 °F

### **Softening Point**

No data available

### **Boiling Point/Range**

304.2±25.0 °C(Predicted)

### **Flash Point**

> 110 °C / > 230 °F Method - No information available

### **Evaporation Rate**

Not applicable Solid

### **Flammability (solid,gas)**

No information available

### **Explosion Limits**

No data available

### **Vapor Pressure**

No data available

### **Vapor Density**

Not applicable Solid

### **Specific Gravity / Density**

1.76±0.1 g/cm<sup>3</sup>(Predicted)

### **Bulk Density**

1.76±0.1 g/cm<sup>3</sup>(Predicted)

### **Water Solubility**

No information available

### **Solubility in other solvents**

No information available

### **Partition Coefficient (n-octanol/water)**

No data available

### **Autoignition Temperature**

No data available

### **Decomposition Temperature**

No data available

### **Viscosity**

Not applicable Solid

### **Explosive Properties**

No information available

### **Oxidizing Properties**

No information available

### **Molecular Formula**

C7 H4 INS

### **Molecular Weight**

261.09

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## SECTION 10: Stability and reactivity

### **Stability**

Moisture sensitive. Light sensitive.

### **Hazardous Reactions**

None under normal processing.

### **Hazardous Polymerization**

No information available.

### **Conditions to Avoid**

None known.

### **Materials to avoid**

No information available.

### **Hazardous Decomposition Products**

Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>). Nitrogen oxides (NO<sub>x</sub>). Sulfur oxides.

Hydrogen iodide.

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## SECTION 11: Toxicological information

### **Product Information**

**(a) acute toxicity;**

**(b) skin corrosion/irritation;**

Category 1 B

**(c) serious eye damage/irritation;**

Category 1

**(d) respiratory or skin sensitization;**

**Respiratory**

No data available

**Skin**

No data available

**(e) germ cell mutagenicity;**

No data available

**(f) carcinogenicity;**

No data available

There are no known carcinogenic chemicals in this product

**(g) reproductive toxicity;**

No data available

**(h) STOT-single exposure;**

No data available

**(i) STOT-repeated exposure;**

No data available

**Target Organs**

No information available.

**(j) aspiration hazard;**

Not applicable

Solid

**Symptoms / effects, both acute and delayed**

Product is a corrosive material. Use of gastric lavage or emesis is contraindicated.

Possible perforation of stomach or esophagus should be investigated: Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation

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## SECTION 12: Ecological information

**Ecotoxicity effects**

Contains no substances known to be hazardous to the environment or that are not degradable in waste water treatment plants.

**Persistence and Degradability**

No information available

**Bioaccumulative Potential**

No information available

**Mobility in soil**

No information available

## Endocrine Disruptor Information

This product does not contain any known or suspected endocrine disruptors

## Persistent Organic Pollutant

This product does not contain any known or suspected substance

## Ozone Depletion Potential

This product does not contain any known or suspected substance

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## SECTION 13: Disposal considerations

### Waste from Residues/Unused Products

Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.

### Contaminated Packaging

Dispose of this container to hazardous or special waste collection point.

### Other Information

Waste codes should be assigned by the user based on the application for which the product was used. Do not empty into drains. Do not flush to sewer. Large amounts will affect pH and harm aquatic organisms.

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## SECTION 14: Transport information

### Road and Rail Transport

#### UN-No

UN2923

#### Proper Shipping Name

Corrosive solid, toxic, n.o.s.

#### Technical Shipping Name

(2-Iodophenyl isothiocy anate)

#### Hazard Class

8

Subsidiary Hazard Class 6.1

#### Packing Group

III

### IMDG/IMO

#### UN-No

UN2923

#### Proper Shipping Name

Corrosive solid, toxic, n.o.s.

**Technical Shipping Name**

(2-Iodophenyl isothiocy anate)

**Hazard Class**

8

Subsidiary Hazard Class 6.1

**Packing Group**

III

**IATA****UN-No**

UN2923

**Proper Shipping Name**

CORROSIVE SOLID, TOXIC, N.O.S.\*

**Technical Shipping Name**

(2-Iodophenyl isothiocy anate)

**Hazard Class**

8

Subsidiary Hazard Class 6.1

**Packing Group**

III

**Special Precautions for User**

No special precautions required

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## SECTION 15: Regulatory information

**International Inventories**

X = listed, China (IECSC), Europe (EINECS/ELINCS/NLP), U.S.A. (TSCA), Canada (DSL/NDL), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), Korea (KECL).

**National Regulations**

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## SECTION 16: Other information

**Prepared By**

Health, Safety and Environmental Department

**Revision Date**

24-Oct-2025

**Revision Summary**

Not applicable.

**Training Advice**

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene. Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

## **Legend**

### **CAS**

Chemical Abstracts Service

### **TSCA**

United States Toxic Substances Control Act Section 8(b)

Inventory

### **EINECS/ELINCS**

European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

### **DSL/NDSL**

Canadian Domestic Substances List/Non-Domestic Substances List

### **PICCS**

Philippines Inventory of Chemicals and Chemical Substances

### **ENCS**

Japanese Existing and New Chemical Substances

### **IECSC**

Chinese Inventory of Existing Chemical Substances

### **AICS**

Australian Inventory of Chemical Substances

### **KECL**

Korean Existing and Evaluated Chemical Substances

### **NZIoC**

New Zealand Inventory of Chemicals

### **WEL**

Workplace Exposure Limit

### **TWA**

Time Weighted Average

### **ACGIH**

American Conference of Governmental Industrial Hygienists

### **IARC**

International Agency for Research on Cancer

### **DNEL**

Derived No Effect Level

### **PNEC**

Predicted No Effect Concentration

### **RPE**

Respiratory Protective Equipment

**LD50**

Lethal Dose 50%

**LC50**

Lethal Concentration 50%

**EC50**

Effective Concentration 50%

**NOEC**

No Observed Effect Concentration

**POW**

Partition coefficient Octanol:Water

**PBT**

Persistent, Bioaccumulative, Toxic

**vPvB**

very Persistent, very Bioaccumulative

**ICAO/IATA**

International Civil Aviation Organization/International Air  
Transport Association

**IMO/IMDG**

International Maritime Organization/International Maritime  
Dangerous Goods Code

**ADR**

European Agreement Concerning the International Carriage of  
Dangerous Goods by Road

**MARPOL**

International Convention for the Prevention of Pollution from  
Ships

**OECD**

Organisation for Economic Co-operation and Development

**ATE**

Acute Toxicity Estimate

**BCF**

Bioconcentration factor

**VOC**

(Volatile Organic Compound)

**Key literature references and sources for data**

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

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