

# SAFETY DATA SHEET

Version 8.8  
Revision Date 09/07/2024  
Print Date 09/14/2024

## SECTION 1: Identification of the substance/mixture and of the company/undertaking

### 1.1 Product identifiers

Product name : Iodobenzene for synthesis  
Product Number : 8.20730  
Catalogue No. : 820730  
Brand : Millipore  
CAS-No. : 591-50-4

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

Identified uses : Chemical for synthesis  
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 4), H227  
Acute toxicity, Oral (Category 4), H302

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

H227

Combustible liquid.

H302

Harmful if swallowed.

Precautionary Statements

P210

Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.

P264

Wash skin thoroughly after handling.

P270

Do not eat, drink or smoke when using this product.

P280

Wear protective gloves/ eye protection/ face protection.

P301 + P312 + P330

IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.

P370 + P378

In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.

P403 + P235

Store in a well-ventilated place. Keep cool.

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>6</sub>H<sub>5</sub>I  
Molecular weight : 204.01 g/mol  
CAS-No. : 591-50-4  
EC-No. : 209-719-6

Component	Classification	Concentration
<b>iodobenzene</b>		
	Flam. Liq. 4; Acute Tox. 4; H227, H302	<= 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.

Millipore - 8.20730

Page 2 of 10

The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada

**MILLIPORE  
SIGMA**

**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. 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****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

Hydrogen iodide

Combustible.

Fire may cause evolution of:

hydrogen iodide

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

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

**5.3 Advice for firefighters**

In the event of fire, wear self-contained breathing apparatus.

**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.

## **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**

Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

For precautions see section 2.2.

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

#### **Storage conditions**

Protected from light. Tightly closed.

Recommended storage temperature see product label.

#### **Storage class**

Storage class (TRGS 510): 10: Combustible liquids

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

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

---

## **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**

Change contaminated clothing. Preventive skin protection recommended. Wash hands 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

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 EN 16523-1 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: Viton®

Minimum layer thickness: 0.7 mm

Break through time: 480 min

Material tested: Vitoject® (KCL 890 / Aldrich Z677698, Size M)

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 EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.4 mm

Break through time: 10 min

Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

### Body Protection

protective clothing

### Respiratory protection

Recommended Filter type: Filter type ABEK

The entrepreneur 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.

---

## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

- |               |                               |
|---------------|-------------------------------|
| a) Appearance | Form: liquid<br>Color: yellow |
| b) Odor       | No data available             |

c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/ range: -29 °C (-20 °F)
f) Initial boiling point and boiling range	188 °C 370 °F at 1,013 hPa 63 - 65 °C (145 - 149 °F) at 13 hPa
g) Flash point	77 °C (171 °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	1.830 g/cm <sup>3</sup>
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

---

## SECTION 10: Stability and reactivity

### 10.1 Reactivity

Forms explosive mixtures with air on intense heating.

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

### 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

Light.  
Strong heating.

#### 10.5 Incompatible materials

Magnesium, Strong oxidizing agents

#### 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

LD50 Oral - Rat - 1,749 mg/kg

Remarks: (RTECS)

LC50 Inhalation - Rat - 16.32 mg/l - dust/mist

Remarks: (RTECS)

Dermal: No data available

##### 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.

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

---

## 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 Endocrine disrupting properties

No data available

### 12.7 Other adverse effects

Discharge into the environment must be avoided.

---

## 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)

Not dangerous goods

Millipore - 8.20730

Page 8 of 10



**IMDG**

Not dangerous goods

**IATA**

Not dangerous goods

**Further information**

Not classified as dangerous in the meaning of transport regulations.

---

**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**

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

**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.

**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

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

TSCA : All substances listed as active on the 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.

---

**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](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact [mlsbranding@sial.com](mailto:mlsbranding@sial.com).

Version: 8.8

Revision Date: 09/07/2024

Print Date: 09/14/2024