

## SAFETY DATA SHEET

Version 8.2  
Revision Date 04/30/2021  
Print Date 05/14/2022**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : 2-Iodoxybenzoic acid

Product Number : 661384  
Brand : Aldrich**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 STATESTelephone : +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 corrosion (Category 1), H314

Serious eye damage (Category 1), H318

Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335

Specific target organ toxicity - repeated exposure, Inhalation (Category 1), Lungs, H372

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 : Danger

Hazard statement(s)  
H314 : Causes severe skin burns and eye damage.

H335 May cause respiratory irritation.  
 H372 Causes damage to organs (Lungs) through prolonged or repeated exposure if inhaled.

Precautionary statement(s)

P260 Do not breathe dust/ fume/ gas/ mist/ vapors/ spray.  
 P264 Wash skin thoroughly after handling.  
 P270 Do not eat, drink or smoke when using this product.  
 P271 Use only outdoors or in a well-ventilated area.  
 P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.  
 P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.  
 P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.  
 P304 + P340 + P310 IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.  
 P305 + P351 + P338 + P310 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor.  
 P314 Get medical advice/ attention if you feel unwell.  
 P363 Wash contaminated clothing 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**

Risk of explosion if heated under confinement.

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

**3.2 Mixtures**

Synonyms : SIBX  
 Stabilized IBX

Molecular weight : 280.02 g/mol

Component	Classification	Concentration
<b>o-Iodoxybenzoic acid</b>		
CAS-No. 61717-82-6	Skin Irrit. 2; Eye Irrit. 2A; STOT SE 3; H315, H319, H335	>= 30 - < 50 %
<b>isophthalic acid</b>		
CAS-No. 121-91-5 EC-No. 204-506-4		>= 30 - < 50 %
<b>Benzoic acid</b>		
CAS-No. 65-85-0 EC-No. 200-618-2 Registration	Skin Irrit. 2; Eye Dam. 1; STOT RE 1; Aquatic Acute 3; H315, H318, H372,	>= 20 - < 30 %

number	01-2119455536-33-XXXX	H402	
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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

First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

#### If inhaled

After inhalation: fresh air. Call in physician.

#### In case of skin contact

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

#### In case of eye contact

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

#### If swallowed

After swallowing: make victim drink water (two glasses at most), avoid vomiting (risk of perforation). Call a physician immediately. Do not attempt to neutralise.

### 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

Hydrogen iodide

Combustible.

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 generation and inhalation of dusts in all circumstances. 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**

#### **Advice on safe handling**

Work under hood. Do not inhale substance/mixture.

#### **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**

Tightly closed. Dry. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

Product is sensitive to light and moisture. Handle and store under inert gas.

Storage class (TRGS 510): 6.1C: Combustible, acute toxic Cat.3 / toxic compounds or compounds which causing chronic effects

### **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
isophthalic acid	121-91-5	TWA	10 mg/m <sup>3</sup>	USA. Workplace Environmental Exposure Levels (WEEL)
		TWA	5 mg/m <sup>3</sup>	USA. Workplace Environmental Exposure Levels (WEEL)

## 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). Tightly fitting safety goggles

#### 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.

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.2 mm

Break through time: 480 min

Material tested: Dermatrill® P (KCL 743 / Aldrich Z677388, Size M)

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.2 mm

Break through time: 480 min

Material tested: Dermatrill® P (KCL 743 / Aldrich Z677388, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

#### Body Protection

Acid-resistant 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: crystalline   |
| b) Odor   | No data available   |
| c) Odor Threshold                               | No data available   |
| d) pH   | 1.8   |
| e) Melting point/freezing point                 | Melting point/range: 250 °C (482 °F) - Decomposes on heating. |
| 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) 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

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

Risk of explosion if heated under confinement.

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) .

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### 10.3 Possibility of hazardous reactions

No data available

### 10.4 Conditions to avoid

no information available

### 10.5 Incompatible materials

Strong bases, Oxidizing agents, Strong oxidizing agents, Strong reducing 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

#### Mixture

#### Acute toxicity

No data available

Symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages:, damage of respiratory tract

Acute toxicity estimate Dermal - > 5,000 mg/kg

(Calculation method)

No data available

#### Skin corrosion/irritation

No data available

#### Serious eye damage/eye irritation

Mixture causes serious eye damage. Risk of blindness!

#### 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

Mixture may cause respiratory irritation.

**Specific target organ toxicity - repeated exposure**

Mixture causes damage to organs through prolonged or repeated exposure. - Lungs

**Aspiration hazard**

No data available

**11.2 Additional Information**

Not available

spasm, inflammation and edema of the larynx, spasm, inflammation and edema of the bronchi, pneumonitis, pulmonary edema, burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

Stomach - Irregularities - Based on Human Evidence

**Components****o-Iodoxybenzoic acid****Acute toxicity**

No data available

Inhalation: No data available

Dermal: No data available

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****Reproductive toxicity**

No data available

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



## isophthalic acid

### Acute toxicity

LD50 Oral - Rat - male and female - > 5,000 mg/kg

(OECD Test Guideline 401)

LC50 Inhalation - Rat - male and female - 4 h - > 11,370 mg/m<sup>3</sup>

(OECD Test Guideline 403)

LD50 Dermal - Rabbit - male and female - > 2,000 mg/kg

(OECD Test Guideline 402)

No data available

### Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 4 h

(OECD Test Guideline 404)

### Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation - 2 s

(OECD Test Guideline 405)

### Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: Does not cause skin sensitization.

(OECD Test Guideline 406)

### Germ cell mutagenicity

Hamster

ovary

Result: negative

### Carcinogenicity

#### Reproductive toxicity

No data available

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

## Benzoic acid

### Acute toxicity

LD50 Oral - Mouse - male and female - 2,250 mg/kg

(OECD Test Guideline 401)

Symptoms: Nausea, Vomiting, Irritation of mucous membranes

LC50 Inhalation - Rat - male and female - 4 h - > 12.2 mg/l

Remarks:

(ECHA)

Symptoms: Cough, Possible damages: , mucosal irritations

LD50 Dermal - Rabbit - male and female - > 2,000 mg/kg

Remarks:

(ECHA)

No data available

#### **Skin corrosion/irritation**

Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

#### **Serious eye damage/eye irritation**

Eyes - Rabbit

Result: Corrosive - 21 Days

(Directive 67/548/EEC, Annex V, B.5.)

(Regulation (EC) No 1272/2008, Annex VI)

#### **Respiratory or skin sensitization**

Local lymph node assay (LLNA) - Mouse

Result: negative

Remarks:

(ECHA)

#### **Germ cell mutagenicity**

Mutagenicity (mammal cell test): chromosome aberration.

Chinese hamster fibroblasts

Result: Positive results were obtained in some in vitro tests.

Remarks:

(ECHA)

Micronucleus test

mouse lymphoma cells

Result: negative

#### **Carcinogenicity**

#### **Reproductive toxicity**

No data available

#### **Specific target organ toxicity - single exposure**

No data available

Acute oral toxicity - Nausea, Vomiting, Irritation of mucous membranes

Acute inhalation toxicity - Cough, Possible damages:, mucosal irritations

#### **Specific target organ toxicity - repeated exposure**

Inhalation - Causes damage to organs through prolonged or repeated exposure. -

Lungs

Remarks:

Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

#### **Aspiration hazard**

No data available

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## **SECTION 12: Ecological information**

### **12.1 Toxicity**

#### **Mixture**

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

### Components

#### **o-Iodoxybenzoic acid**

No data available

#### **isophthalic acid**

Toxicity to fish	static test LC50 - <i>Leuciscus idus melanotus</i> - > 907 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - <i>Daphnia magna</i> (Water flea) - > 952 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	static test ErC50 - <i>Desmodesmus subspicatus</i> (green algae) - > 1,000 mg/l - 96 h (OECD Test Guideline 201)
Toxicity to bacteria	Respiration inhibition EC50 - Sludge Treatment - 617.1 mg/l - 3 h (OECD Test Guideline 209)

#### **Benzoic acid**

Toxicity to fish	static test LC50 - <i>Lepomis macrochirus</i> - 44.6 mg/l - 96 h (US-EPA)
Toxicity to daphnia and other aquatic invertebrates	static test LC50 - <i>Daphnia magna</i> (Water flea) - > 100 mg/l - 48 h (US-EPA)
Toxicity to algae	static test ErC50 - <i>Pseudokirchneriella subcapitata</i> - > 33.1 mg/l - 72 h (OECD Test Guideline 201)
Toxicity to bacteria	static test IC50 - activated sludge - > 1,000 mg/l - 3 h (OECD Test Guideline 209)  microtox test EC50 - <i>Photobacterium phosphoreum</i> - 17 mg/l - 30 min Remarks: (Lit.)

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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)

UN number: 1759 Class: 8 Packing group: II  
Proper shipping name: Corrosive solids, n.o.s. (isophthalic acid, o-Iodoxybenzoic acid)  
Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

#### IMDG

UN number: 1759 Class: 8 Packing group: II EMS-No: F-A, S-B  
Proper shipping name: CORROSIVE SOLID, N.O.S. (isophthalic acid, o-Iodoxybenzoic acid)

#### IATA

UN number: 1759 Class: 8 Packing group: II  
Proper shipping name: Corrosive solid, n.o.s. (isophthalic acid, o-Iodoxybenzoic acid)

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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

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.

#### SARA 311/312 Hazards

Acute Health Hazard, Chronic 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

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Version: 8.2

Revision Date: 04/30/2021

Print Date: 05/14/2022