

SAFETY DATA SHEET

Version 8.9
Revision Date 09/08/2024
Print Date 09/09/2024

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

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)**

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.

Aldrich - 661384

Page 1 of 14

2.2 GHS Label elements, including precautionary statements

Pictogram



Signal Word

Danger

Hazard Statements

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 Statements

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 |
|-----------------------------|---|----------------|
| o-Iodoxybenzoic acid | | |
| CAS-No. 61717-82-6 | Skin Irrit. 2; Eye Irrit. 2A; STOT SE 3; H315, H319, H335 | >= 30 - < 50 % |

Aldrich - 661384

Page 2 of 14

| | | | |
|-------------------------|-----------------------|---|----------------|
| isophthalic acid | | | |
| CAS-No. | 121-91-5 | | >= 30 - < 50 % |
| EC-No. | 204-506-4 | | |
| Benzoic acid | | | |
| CAS-No. | 65-85-0 | Skin Irrit. 2; Eye Dam. 1; STOT RE 1; Aquatic Acute 3; H315, H318, H372, H402 | >= 20 - < 30 % |
| EC-No. | 200-618-2 | | |
| Index-No. | 607-705-00-8 | | |
| Registration number | 01-2119455536-33-XXXX | | |
| | | | |

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

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

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Water Foam Carbon dioxide (CO2) Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

Aldrich - 661384

Page 3 of 14

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.

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.

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

Aldrich - 661384

Page 4 of 14

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

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 ³ | USA. Workplace Environmental Exposure Levels (WEEL) |
| | | TWA | 5 mg/m ³ | USA. Workplace Environmental Exposure Levels (WEEL) |
| Benzoic acid | 65-85-0 | TWA | 0.5 mg/m ³ | USA. ACGIH Threshold Limit Values (TLV) |
| | Remarks | Not suspected as a human carcinogen Danger of cutaneous absorption | | |

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: Dermatril® 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: Dermatril® 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

Recommended Filter type: Filter type P2

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 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.

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) Density | No data available |
| 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 | Not classified as explosive. |
| t) Oxidizing properties | none |

9.2 Other safety information

No data available

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) .

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

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Mixture

Acute toxicity

Oral: 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)

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

Remarks: 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

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

Oral: No data available

Aldrich - 661384

Page 8 of 14

Inhalation: No data available
Dermal: No data available
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

No data available

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/m³ - dust/mist

(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

Test Type: Hamster

Test system: ovary

Result: negative

Carcinogenicity

No data available

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 - dust/mist

Remarks: (ECHA)

Symptoms: Cough, Possible damages:, mucosal irritations

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

Remarks: (ECHA)

Skin corrosion/irritation

Skin - Guinea pig

Result: Skin irritation - 3 h

Remarks: (ECHA)

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

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Corrosive - 21 Days

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

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

Respiratory or skin sensitization

Local lymph node assay (LLNA) - Mouse

Result: negative

Remarks: (ECHA)

Germ cell mutagenicity

Test Type: Mutagenicity (mammal cell test): chromosome aberration.

Test system: Chinese hamster fibroblasts

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

Remarks: (ECHA)

Test Type: Micronucleus test

Test system: mouse lymphoma cells

Result: negative

Carcinogenicity

No data available

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

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

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 Endocrine disrupting properties

No data available

12.7 Other adverse effects

No data available

Components**o-Iodoxybenzoic acid**

No data available

Aldrich - 661384

Page 11 of 14

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.) |
| Toxicity to fish(Chronic toxicity) | semi-static test EC50 - <i>Oncorhynchus mykiss</i> (rainbow trout) - > 120 mg/l - 28 d (OECD Test Guideline 204) |
| Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity) | semi-static test EC50 - <i>Daphnia magna</i> (Water flea) - > 25 mg/l - 21 d (OECD Test Guideline 211) |

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

SECTION 15: Regulatory information

CERCLA Reportable Quantity

| Components | CAS-No. | Component RQ (lbs) | Calculated product RQ (lbs) |
|--------------|---------|--------------------|-----------------------------|
| Benzoic acid | 65-85-0 | 5000 | |

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 311/312 Hazards : Acute Health Hazard
Chronic 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

Benzoic acid 65-85-0

Pennsylvania Right To Know

Benzoic acid 65-85-0

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 : 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.

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.

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.

Version: 8.9

Revision Date: 09/08/2024

Print Date: 09/09/2024