

SAFETY DATA SHEET

Version 9.0
Revision Date 09/30/2024
Print Date 10/01/2024

SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1 Product identifiers**

Product name : Phenylzinc iodide solution

Product Number : 499331
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)**

Flammable liquids (Category 2), H225
Chemicals which, in contact with water, emit flammable gases (Category 2), H261
Acute toxicity, Oral (Category 4), H302
Skin irritation (Category 2), H315
Eye irritation (Category 2A), H319

Carcinogenicity (Category 2), H351

Specific target organ toxicity - single exposure (Category 3), Respiratory system, Central nervous system, H335, H336

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 Statements

| | |
|------|---|
| H225 | Highly flammable liquid and vapor. |
| H261 | In contact with water releases flammable gas. |
| H302 | Harmful if swallowed. |
| H315 | Causes skin irritation. |
| H319 | Causes serious eye irritation. |
| H335 | May cause respiratory irritation. |
| H336 | May cause drowsiness or dizziness. |
| H351 | Suspected of causing cancer. |

Precautionary Statements

| | |
|--------------------|--|
| P201 | Obtain special instructions before use. |
| P202 | Do not handle until all safety precautions have been read and understood. |
| P210 | Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking. |
| P223 | Do not allow contact with water. |
| P231 + P232 | Handle under inert gas. Protect from moisture. |
| 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. |
| 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 + P312 + P330 | IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth. |
| 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. |
| P308 + P313 | IF exposed or concerned: Get medical advice/ attention. |
| P332 + P313 | If skin irritation occurs: Get medical advice/ attention. |
| P335 + P334 | Brush off loose particles from skin. Immerse in cool water/ wrap |

| | |
|-------------|--|
| P337 + P313 | in wet bandages. |
| P362 | If eye irritation persists: Get medical advice/ attention. |
| P370 + P378 | Take off contaminated clothing and wash before reuse. |
| | In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish. |
| P402 + P404 | Store in a dry place. Store in a closed container. |
| 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

May form explosive peroxides.

SECTION 3: Composition/information on ingredients

3.2 Mixtures

Formula : C_6H_5IZn
Molecular weight : 269.40 g/mol

| Component | | Classification | Concentration |
|--------------------------|-----------------------|---|-------------------|
| Tetrahydrofuran | | | |
| CAS-No. | 109-99-9 | Flam. Liq. 2; Acute Tox. 4; Eye Irrit. 2A; Carc. 2; STOT SE 3; H225, H302, H319, H351, H335, H336 Concentration limits: >= 25 %: Eye Irrit. 2, H319; >= 25 %: STOT SE 3, H335; | >= 70 - < 90 % |
| EC-No. | 5-53 | | |
| Index-No. | 603-025-00-0 | | |
| Registration number | 01-2119444314-46-XXXX | | |
| Phenylzinc iodide | | | |
| CAS-No. | 23665-09-0 | Acute Tox. 4; Skin Irrit. 2; Eye Irrit. 2A; STOT SE 3; H302, H315, H319, H335 | >= 10 - < 20 % |

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. Call in physician.

In case of skin contact

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

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****Suitable extinguishing media**

Carbon dioxide (CO₂) Dry powder

Unsuitable extinguishing media

Water Foam

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Hydrogen iodide

Zinc/zinc oxides

Combustible.

Pay attention to flashback.

Vapors are heavier than air and may spread along floors.

May not get in touch with: Water

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

Forms explosive mixtures with air at ambient 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 carefully 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 safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols. Keep workplace dry. Do not allow product to come into contact with water.

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

Tightly closed. Keep away from heat and sources of ignition. Never allow product to get in contact with water during storage.

Storage stability Recommended storage temperature

2 - 8 °C

Store under inert gas. Test for peroxide formation periodically and before distillation.

Storage class

Storage class (TRGS 510): 4.3: Hazardous materials, which set free flammable gases upon contact with water

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 |
|-----------------|----------|--|----------------------|---|
| Tetrahydrofuran | 109-99-9 | TWA | 50 ppm | USA. ACGIH Threshold Limit Values (TLV) |
| | Remarks | Confirmed animal carcinogen with unknown relevance to humans Danger of cutaneous absorption | | |
| | | STEL | 100 ppm | USA. ACGIH Threshold Limit Values (TLV) |
| | | Confirmed animal carcinogen with unknown relevance to humans Danger of cutaneous absorption | | |
| | | ST | 250 ppm 735 mg/m3 | USA. NIOSH Recommended Exposure Limits |
| | | TWA | 200 ppm 590 mg/m3 | USA. NIOSH Recommended Exposure Limits |
| | | TWA | 200 ppm 590 mg/m3 | USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants |
| | | PEL | 200 ppm 590 mg/m3 | California permissible exposure limits for chemical contaminants (Title 8, Article 107) |
| | | STEL | 250 ppm 735 mg/m3 | California permissible exposure limits for chemical contaminants (Title 8, Article 107) |

Biological occupational exposure limits

| Component | CAS-No. | Parameters | Value | Biological specimen | Basis |
|-----------------|----------|--|--------|---------------------|---|
| Tetrahydrofuran | 109-99-9 | Tetrahydrofuran | 2 mg/l | Urine | ACGIH - Biological Exposure Indices (BEI) |
| | Remarks | End of shift (As soon as possible after exposure ceases) | | | |

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 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. Risk of explosion.

SECTION 9: Physical and chemical properties**9.1 Information on basic physical and chemical properties**

| | |
|---|-----------------------------|
| a) Appearance | Form: liquid |
| b) Odor | No data available |
| c) Odor Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | No data available |
| f) Initial boiling point and boiling range | No data available |
| g) Flash point | -17 °C (1 °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 | 0.966 g/mL at 25 °C (77 °F) |
| Relative density | No data available |
| n) Water solubility | No data available |
| o) Partition coefficient: n-octanol/water | No data available |

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- | | |
|------------------------------|------------------------------|
| 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

Formation of peroxides possible.
Vapors may form explosive mixture with air.

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

Warming.
Moisture.

10.5 Incompatible materials

Bases, Oxidizing agents, Oxygen, acids

10.6 Hazardous decomposition products

Peroxides
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

Acute toxicity estimate Oral - 1,229 mg/kg

(Calculation method)

Symptoms: Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.

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

Dermal: No data available

Acute toxicity estimate Dermal - 2,938 mg/kg
(Calculation method)

Skin corrosion/irritation

Remarks: Mixture causes skin irritation.

Serious eye damage/eye irritation

Remarks: Mixture causes serious eye irritation.

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

Evidence of a carcinogenic effect.

IARC: 2B - Group 2B: Possibly carcinogenic to humans (Tetrahydrofuran)

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.

Mixture may cause drowsiness or dizziness.

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., 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, Nausea
Other dangerous properties can not be excluded.

This substance should be handled with particular care.

Handle in accordance with good industrial hygiene and safety practice.

Stomach - Irregularities - Based on Human Evidence

Components

Tetrahydrofuran

Acute toxicity

LD50 Oral - Rat - male and female - 1,650 mg/kg

Remarks: (ECHA)

Symptoms: Irritation of mucous membranes

LC50 Inhalation - Rat - male and female - 6 h - > 14.7 mg/l - vapor
(US-EPA)

LD50 Dermal - Rat - male and female - > 2,000 mg/kg
(OECD Test Guideline 402)

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 72 h

(Draize Test)

Remarks: Repeated or prolonged exposure may cause skin irritation and dermatitis, due to degreasing properties of the product.

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Causes serious eye irritation.

Remarks: (IUCLID)

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

Respiratory or skin sensitization

Local lymph node assay (LLNA) - Mouse

Result: negative

(OECD Test Guideline 429)

Germ cell mutagenicity

Test Type: Ames test

Test system: *S. typhimurium*

Result: negative

Test Type: In vitro mammalian cell gene mutation test

Test system: Chinese hamster ovary cells

Result: negative

Test Type: Chromosome aberration test in vitro

Test system: Chinese hamster ovary cells

Result: negative

Method: OECD Test Guideline 474

Species: Mouse - male and female - Red blood cells (erythrocytes)

Result: negative

Carcinogenicity

Suspected of causing cancer.

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

Inhalation - May cause respiratory irritation. - Central nervous system

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

May cause drowsiness or dizziness.
Acute oral toxicity - Irritation of mucous membranes

Specific target organ toxicity - repeated exposure

Aspiration hazard

No data available

Phenylzinc iodide

Acute toxicity

Oral: No data available
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

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

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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

Tetrahydrofuran

| | |
|---|--|
| Toxicity to fish | flow-through test LC50 - Pimephales promelas (fathead minnow) - 2,160 mg/l - 96 h (OECD Test Guideline 203) |
| Toxicity to daphnia and other aquatic invertebrates | static test EC50 - Daphnia magna (Water flea) - 3,485 mg/l - 48 h (OECD Test Guideline 202) |
| Toxicity to fish(Chronic toxicity) | flow-through test NOEC - Pimephales promelas (fathead minnow) - 216 mg/l - 33 d Remarks: (ECHA) |

Phenylzinc iodide

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: 3399 Class: 4.3 (3) Packing group: II
Proper shipping name: Organometallic substance, liquid, water-reactive, flammable
(Phenylzinc iodide, Tetrahydrofuran) (Phenylzinc iodide, Tetrahydrofuran)

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Reportable Quantity (RQ): 1175 lbs
Poison Inhalation Hazard: No

IMDG

UN number: 3399 Class: 4.3 (3) Packing group: II EMS-No: F-G, S-N
Proper shipping name: ORGANOMETALLIC SUBSTANCE, LIQUID, WATER-REACTIVE,
FLAMMABLE (Tetrahydrofuran, Phenylzinc iodide) (Tetrahydrofuran, Phenylzinc iodide)

IATA

UN number: 3399 Class: 4.3 (3) Packing group: II
Proper shipping name: Organometallic substance, liquid, water-reactive, flammable
(Tetrahydrofuran, Phenylzinc iodide) (Tetrahydrofuran, Phenylzinc iodide)

SECTION 15: Regulatory information

CERCLA Reportable Quantity

| Components | CAS-No. | Component RQ (lbs) | Calculated product RQ (lbs) |
|-----------------|----------|-----------------------|--------------------------------|
| Tetrahydrofuran | 109-99-9 | 1000 | 1175 |

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
Reactivity Hazard
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

Tetrahydrofuran 109-99-9

Pennsylvania Right To Know

Tetrahydrofuran 109-99-9

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

California Prop. 65

WARNING: This product can expose you to chemicals including Tetrahydrofuran, which is/are known to the State of California to cause cancer. For more information go to www.P65Warnings.ca.gov.

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**Relevant changes since previous version**

5. Fire-fighting measures

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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