

SAFETY DATA SHEET

Revision Date 01-April-2024 Revision Number 4

1. Identification

Product Name 3-(Ethoxycarbonyl)phenylzinc iodide, 0.5M in THF

Cat No.: H58105

Synonyms No information available

Recommended Use Laboratory chemicals.

Uses advised against Food, drug, pesticide or biocidal product use.

Details of the supplier of the safety data sheet

Company

Importer/Distributor

Fisher Scientific 112 Colonnade Road, Ottawa, ON K2E 7L6,

Canada

Tel: 1-800-234-7437

Emergency Telephone Number

For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11 Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99 **CHEMTREC** Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

2. Hazard(s) identification

Classification

WHMIS 2015 Classification Classified as hazardous under the Hazardous Products Regulations (SOR/2015-17)

Flammable liquids
Category 2
Acute oral toxicity
Category 4
Skin Corrosion/Irritation
Carcinogenicity
Carcinogenicity
Carcinogenicity
Category 1
Carcinogenicity
Category 2
Specific target organ toxicity (single exposure)
Category 3
Target Organs - Respiratory system, Central nervous system (CNS).
Physical Hazards Not Otherwise Classified
Category 1

May form explosive peroxides

Label Elements

Signal Word

Danger

Hazard Statements

Highly flammable liquid and vapor
Harmful if swallowed
Causes severe skin burns and eye damage
May cause respiratory irritation
May cause drowsiness and dizziness
Suspected of causing cancer
May form explosive peroxides



Precautionary Statements

Prevention

Obtain special instructions before use

Do not handle until all safety precautions have been read and understood

Wear protective gloves/protective clothing/eye protection/face protection

Keep container tightly closed

Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking

Ground/bond container and receiving equipment

Do not breathe dust/fumes/gas/mist/vapours/spray

Wash face, hands and any exposed skin thoroughly after handling

Do not eat, drink or smoke when using this product

Use only outdoors or in a well-ventilated area

Use non-sparking tools

Take action to prevent static discharges

Response

IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower

IF INHALED: Remove person to fresh air and keep comfortable for breathing

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

Rinse mouth

Do NOT induce vomiting

Wash contaminated clothing before reuse

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

Storage

Store locked up

Store in a well-ventilated place. Keep container tightly closed

Disposal

Dispose of contents/container to an approved waste disposal plant

3. Composition/Information on Ingredients

| Component | CAS-No | Weight % | |
|-------------------------------------|-------------|----------|--|
| Tetrahydrofuran | 109-99-9 | 83 | |
| 3-(Ethoxycarbonyl)phenylzinc iodide | 282727-18-8 | 17 | |

4. First-aid measures

General Advice

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

Eye ContactRinse immediately with plenty of water, also under the eyelids, for at least 15 minutes.

Immediate medical attention is required.

Skin Contact Wash off immediately with plenty of water for at least 15 minutes. Remove and wash

contaminated clothing and gloves, including the inside, before re-use. Call a physician

immediately.

Inhalation If not breathing, give artificial respiration. Remove from exposure, lie down. 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. Call a physician immediately.

Ingestion Do NOT induce vomiting. Clean mouth with water. Never give anything by mouth to an

unconscious person. Call a physician immediately.

swelling, severe damage to the delicate tissue and danger of perforation: Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting: Product is a corrosive material. Use of gastric lavage or emesis is

contraindicated. Possible perforation of stomach or esophagus should be investigated

Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media Dry sand. Carbon dioxide (CO2). Powder. Do not use water or foam. CO2, dry chemical,

dry sand, alcohol-resistant foam. Water mist may be used to cool closed containers.

Unsuitable Extinguishing Media No information available

Flash Point -17 °C / 1.4 °F

Method - No information available

Autoignition Temperature

Explosion Limits

Notes to Physician

No information available

Upper No data available
Lower No data available
Sensitivity to Mechanical Impact No information available

Sensitivity to Mechanical Impact No information available Sensitivity to Static Discharge No information available

Specific Hazards Arising from the Chemical

Thermal decomposition can lead to release of irritating gases and vapors. The product causes burns of eyes, skin and mucous membranes. Flammable. Containers may explode when heated. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back.

Hazardous Combustion Products

Carbon monoxide (CO). Carbon dioxide (CO2). Hydrogen iodide. Metal oxides.

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

HealthFlammabilityInstabilityPhysical hazards332W

6. Accidental release measures

Personal Precautions Ensure adequate ventilation. Use personal protective equipment as required. Evacuate

personnel to safe areas. Keep people away from and upwind of spill/leak. Remove all

Environmental Precautions

sources of ignition. Take precautionary measures against static discharges. Should not be released into the environment. See Section 12 for additional Ecological Information. Do not allow material to contaminate ground water system. Do not flush into surface water or sanitary sewer system.

Methods for Containment and Clean Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment.

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 mist/vapors/spray. Do not ingest. If swallowed then seek immediate medical assistance. If peroxide formation is suspected, do not open or move container. Keep away from open flames, hot surfaces and sources of ignition. Use only non-sparking tools. To avoid ignition of vapors by static electricity discharge, all metal parts of the equipment must be grounded. Take precautionary measures against static discharges.

Storage.

Keep refrigerated. Corrosives area. Keep containers tightly closed in a dry, cool and well-ventilated place. Containers should be dated when opened and tested periodically for the presence of peroxides. Should crystals form in a peroxidizable liquid, peroxidation may have occurred and the product should be considered extremely dangerous. In this instance. the container should only be opened remotely by professionals. Keep away from heat. sparks and flame. Incompatible Materials. Strong bases. Oxidizing agent.

8. Exposure controls / personal protection

Exposure Guidelines

| Component | Alberta | British | Ontario TWAEV | Quebec | ACGIH TLV | OSHA PEL | NIOSH |
|-----------------|---------------|---------------|---------------|--------------|---------------|-----------------------|---------------|
| | | Columbia | | | | | |
| Tetrahydrofuran | TWA: 50 ppm | TWA: 50 ppm | TWA: 50 ppm | TWA: 100 ppm | TWA: 50 ppm | (Vacated) TWA: | |
| | TWA: 147 | STEL: 100 ppm | STEL: 100 ppm | TWA: 300 | STEL: 100 ppm | 200 ppm | TWA: 200 ppm |
| | mg/m³ | Skin | Skin | mg/m³ | Skin | (Vacated) TWA: | TWA: 590 |
| | STEL: 100 ppm | | | | | 590 mg/m ³ | mg/m³ |
| | STEL: 295 | | | | | (Vacated) STEL: | STEL: 250 ppm |
| | mg/m³ | | | | | 250 ppm | STEL: 735 |
| | Skin | | | | | (Vacated) STEL: | mg/m³ |
| | | | | | | 735 mg/m ³ | |
| | | | | | | TWA: 200 ppm | |
| | | | | | | TWA: 590 | |
| | | | | | | mg/m³ | |

Legend

ACGIH - American Conference of Governmental Industrial Hygienists

OSHA - Occupational Safety and Health Administration

NIOSH: NIOSH - National Institute for Occupational Safety and Health

Engineering Measures

Ensure that eyewash stations and safety showers are close to the workstation location. Ensure adequate ventilation, especially in confined areas. Use explosion-proof

electrical/ventilating/lighting/equipment.

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

Hand Protection Wear appropriate protective gloves and clothing to prevent skin exposure.

| Г | Glove material | Breakthrough time | Glove thickness | Glove comments |
|---|----------------|-------------------|-----------------|------------------------|
| | Nitrile rubber | See manufacturers | - | Splash protection only |
| | Viton (R) | recommendations | | |
| | Butyl rubber | | | |

Inspect gloves before use. observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information) gloves are suitable for the task: Chemical compatability, 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. gloves with care avoiding skin contamination.

Respiratory Protection

When workers are facing concentrations above the exposure limit they must use appropriate certified respirators. Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced. To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly **Recommended Filter type:** low boiling organic solvent Type AX Brown conforming to EN371 or Organic gases and vapours filter Type A Brown conforming to EN14387

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

Environmental exposure controls

No information available.

Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Wash hands before breaks and after work.

9. Physical and chemical properties

Physical State Liquid

AppearanceYellow - Brown - BlackOdorNo information availableOdor ThresholdNo information available

pH No information available
Melting Point/Range No data available
Boiling Point/Range No information available

Flash Point

-17 °C / 1.4 °F

Evaporation Rate

No information available

No information available

Flammability (solid,gas) Not applicable

Flammability or explosive limits

Upper
LowerNo data available
No data availableVapor PressureNo information availableVapor DensityNo information available

Specific Gravity 0.991 g/cm3

Solubility

No information available

Partition coefficient; n-octanol/water

No data available

Autoignition Temperature

No information available

Decomposition Temperature

No information available

Viscosity No information available

Molecular FormulaC9 H9 IO2 ZnMolecular Weight341.45

10. Stability and reactivity

Reactive Hazard None known, based on information available

Stability Air sensitive.

Conditions to Avoid Keep away from open flames, hot surfaces and sources of ignition.

Incompatible Materials Strong bases, Oxidizing agent

Hazardous Decomposition Products Carbon monoxide (CO), Carbon dioxide (CO2), Hydrogen iodide, Metal oxides

Hazardous Polymerization Hazardous polymerization does not occur.

Hazardous Reactions None under normal processing.

11. Toxicological information

Acute Toxicity

Product Information

Oral LD50 Category 4. ATE = 300 - 2000 mg/kg.

Based on ATE data, the classification criteria are not met. ATE > 2000 mg/kg. **Dermal LD50** Vapor LC50 Based on ATE data, the classification criteria are not met. ATE > 20 mg/l.

Component Information

| Component | LD50 Oral | LD50 Dermal | LC50 Inhalation | |
|-----------------|--------------------|-----------------------|-----------------------|--|
| Tetrahydrofuran | 1650 mg/kg (Rat) | > 2000 mg/kg (Rabbit) | 180 mg/L (Rat) 1 h | |
| | | | 53.9 mg/L (Rat) 4 h | |

Toxicologically Synergistic

No information available

Products

Delayed and immediate effects as well as chronic effects from short and long-term exposure

No information available Irritation

Sensitization No information available

Limited evidence of a carcinogenic effect. The table below indicates whether each agency Carcinogenicity

has listed any ingredient as a carcinogen.

| Component | CAS-No | IARC | NTP | ACGIH | OSHA | Mexico |
|-----------------------|-------------|------------|------------|------------|------------|------------|
| Tetrahydrofuran | 109-99-9 | Group 2B | Not listed | A3 | X | A3 |
| 3-(Ethoxycarbonyl)phe | 282727-18-8 | Not listed |
| nylzinc iodide | | | | | | |

IARC (International Agency for Research on Cancer)

IARC (International Agency for Research on Cancer)

Group 1 - Carcinogenic to Humans

Group 2A - Probably Carcinogenic to Humans

Group 2B - Possibly Carcinogenic to Humans

ACGIH: (American Conference of Governmental Industrial A1 - Known Human Carcinogen

A2 - Suspected Human Carcinogen

A3 - Animal Carcinogen

ACGIH: (American Conference of Governmental Industrial Hygienists)

No information available **Mutagenic Effects**

Reproductive Effects No information available. **Developmental Effects** No information available.

No information available. **Teratogenicity**

STOT - single exposure Respiratory system Central nervous system (CNS)

STOT - repeated exposure None known

Aspiration hazard No information available

delayed

Hygienists)

Symptoms / effects, both acute and Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation: Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting: Product is a corrosive material. Use of gastric lavage or emesis is contraindicated. Possible perforation of stomach or esophagus should

be investigated

Endocrine Disruptor Information

| Component | Component EU - Endocrine Disrupters Candidate List | | Japan - Endocrine Disruptor Information |
|-----------------|--|----------------|--|
| Tetrahydrofuran | Group III Chemical | Not applicable | Not applicable |

Other Adverse Effects

The toxicological properties have not been fully investigated.

12. Ecological information

Ecotoxicity

May cause long-term adverse effects in the environment. Do not allow material to contaminate ground water system.

| Component | Freshwater Algae | Freshwater Fish | Microtox | Water Flea |
|-----------------|------------------|----------------------------|------------|-----------------------|
| Tetrahydrofuran | Not listed | 2160 mg/l LC50 = 96 h | Not listed | EC50 48 h 3485 mg/l |
| | | Pimephales promelas | | EC50: >10000 mg/L/24h |
| | | Leuciscus idus: LC50: 2820 | | |
| | | mg/L/48h | | |

Persistence and Degradability

May persist based on information available.

Bioaccumulation/ Accumulation

No information available.

Mobility

Is not likely mobile in the environment due its low water solubility.

| Component | log Pow |
|-----------------|---------|
| Tetrahydrofuran | 0.45 |

13. Disposal considerations

Waste Disposal Methods

Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

| Component | RCRA - U Series Wastes | RCRA - P Series Wastes | |
|----------------------------|------------------------|------------------------|--|
| Tetrahydrofuran - 109-99-9 | U213 | - | |

14. Transport information

DOT

UN-No UN3399

Proper Shipping Name ORGANOMETALLIC SUBSTANCE, LIQUID, WATER-REACTIVE, FLAMMABLE

Technical Name (3-(Ethoxycarbonyl)phenylzinc iodide, TETRAHYDROFURAN)

Hazard Class 4.3
Subsidiary Hazard Class 3
Packing Group II

TDG

UN-No UN3399

Proper Shipping Name Organometallic substance, liquid, water-reactive, flammable

Hazard Class 4.3 Subsidiary Hazard Class 3 Packing Group II

<u>IATA</u>

UN-No UN3399

Proper Shipping Name Organometallic substance, liquid, water-reactive, flammable

Hazard Class 4.3
Subsidiary Hazard Class 3
Packing Group

IMDG/IMO

UN-No UN3399

Proper Shipping Name ORGANOMETALLIC SUBSTANCE, LIQUID, WATER-REACTIVE, FLAMMABLE

Hazard Class 4.3 Subsidiary Hazard Class 3 Packing Group II

15. Regulatory information

International Inventories

| Component | CAS-No | DSL | NDSL | TSCA | TSCA Inventory notification - Active-Inactive | EINECS | ELINCS | NLP |
|-------------------------------------|-------------|-----|------|------|---|-----------|--------|-----|
| Tetrahydrofuran | 109-99-9 | Х | - | Х | ACTIVE | 203-726-8 | - | - |
| 3-(Ethoxycarbonyl)phenylzinc iodide | 282727-18-8 | - | - | - | - | - | - | - |

| Component | CAS-No | IECSC | KECL | ENCS | ISHL | TCSI | AICS | NZIoC | PICCS |
|------------------------------|-------------|-------|----------|------|------|------|------|-------|-------|
| Tetrahydrofuran | 109-99-9 | X | KE-33454 | X | Х | X | X | Х | Χ |
| 3-(Ethoxycarbonyl)phenylzinc | 282727-18-8 | - | - | - | - | - | - | - | - |
| l iodide | | | | | | | | | |

Legend:

X - Listed '-' - Not Listed

KECL - NIER number or KE number (http://ncis.nier.go.kr/en/main.do)

DSL/NDSL - Canadian Domestic Substances List/Non-Domestic Substances List

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

IECSC - Chinese Inventory of Existing Chemical Substances

KECL - Korean Existing and Evaluated Chemical Substances

ENCS - Japanese Existing and New Chemical Substances

AICS - Australian Inventory of Chemical Substances

PICCS - Philippines Inventory of Chemicals and Chemical Substances

Canada

SDS in compliance with provisions of information as set out in Canadian Standard - Part 4, Schedule 1 and 2 of the Hazardous Products Regulations (HPR) and meets the requirements of the HPR (Paragraph 13(1)(a) of the Hazardous Products Act (HPA)).

| Component | Canada - National Pollutant Release Inventory (NPRI) | Canadian Environmental Protection Agency (CEPA) - List of Toxic Substances | Canada's Chemicals Management Plan (CEPA) | |
|-----------------|---|--|--|--|
| Tetrahydrofuran | Part 5, Individual Substances Part 4 Substance | | | |

Legend

NPRI - National Pollutant Release Inventory

Other International Regulations

Authorisation/Restrictions according to EU REACH

| Component | _ (| REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances | |
|-----------------|-----|---|---|
| Tetrahydrofuran | - | Use restricted. See item 75. | - |
| | | (see link for restriction details) | |

REACH links

https://echa.europa.eu/substances-restricted-under-reach

Safety, health and environmental regulations/legislation specific for the substance or mixture

| Component | CAS-No | OECD HPV | Persistent Organic Pollutant | Ozone Depletion Potential | Restriction of Hazardous Substances (RoHS) |
|-------------------------------------|-------------|----------------|---------------------------------|------------------------------|--|
| Tetrahydrofuran | 109-99-9 | Listed | Not applicable | Not applicable | Not applicable |
| 3-(Ethoxycarbonyl)phenylzinc iodide | 282727-18-8 | Not applicable | Not applicable | Not applicable | Not applicable |

| Component | CAS-No | Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification | Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements | Rotterdam Convention (PIC) | Basel Convention (Hazardous Waste) |
|-------------------------------------|-------------|---|--|-------------------------------|---------------------------------------|
| Tetrahydrofuran | 109-99-9 | Not applicable | Not applicable | Not applicable | Not applicable |
| 3-(Ethoxycarbonyl)phenylzinc iodide | 282727-18-8 | Not applicable | Not applicable | Not applicable | Not applicable |

16. Other information

Prepared By Product Safety Department

Email: chem.techinfo@thermofisher.com

www.thermofisher.com

Revision Date 01-April-2024 Print Date 01-April-2024

Revision Summary New emergency telephone response service provider.

Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

End of SDS