

SAFETY DATA SHEET

Revision Date 01-Apr-2024

Revision Number 4

1. Identification

Product Name 4-(Ethoxycarbonyl)phenylzinc iodide, 0.5M in THF

Cat No. : H58484

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

Thermo Fisher Scientific Chemicals, Inc.
30 Bond Street
Ward Hill, MA 01835-8099
Tel: 800-343-0660
Fax: 800-322-4757

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

This chemical is considered hazardous by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

Flammable liquids	Category 2
Substances/mixtures which, in contact with water, emit flammable gases	Category 1
Acute oral toxicity	Category 4
Skin Corrosion/Irritation	Category 1 B
Serious Eye Damage/Eye Irritation	Category 1
Carcinogenicity	Category 2
Specific target organ toxicity (single exposure)	Category 3
Target Organs - Respiratory system, Central nervous system (CNS).	

Label Elements

Signal Word

Danger

Hazard Statements

Highly flammable liquid and vapor
In contact with water releases flammable gases which may ignite spontaneously
Harmful if swallowed
Causes severe skin burns and eye damage
May cause respiratory irritation
May cause drowsiness or dizziness
Suspected of causing cancer

**Precautionary Statements****Prevention**

Obtain special instructions before use
Do not handle until all safety precautions have been read and understood
Use personal protective equipment as required
Wash face, hands and any exposed skin thoroughly after handling
Do not eat, drink or smoke when using this product
Do not breathe dust/fume/gas/mist/vapors/spray
Use only outdoors or in a well-ventilated area
Keep away from heat/sparks/open flames/hot surfaces. - No smoking
Keep container tightly closed
Ground/bond container and receiving equipment
Use explosion-proof electrical/ventilating/lighting equipment
Use only non-sparking tools
Take precautionary measures against static discharge
Keep away from any possible contact with water, because of violent reaction and possible flash fire
Handle under inert gas. Protect from moisture
Keep cool

Response

Immediately call a POISON CENTER or doctor/physician

Inhalation

IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing

Skin

IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower
Wash contaminated clothing before reuse
Brush off loose particles from skin. Immerse in cool water/wrap with wet bandages

Eyes

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing

Ingestion

Rinse mouth
Do NOT induce vomiting

Fire

In case of fire: Use CO₂, dry chemical, or foam for extinction

Storage

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

Disposal

Dispose of contents/container to an approved waste disposal plant

Hazards not otherwise classified (HNOC)

May form explosive peroxides
WARNING. Cancer - <https://www.p65warnings.ca.gov/>.

3. Composition/Information on Ingredients

Component	CAS No	Weight %
Tetrahydrofuran	109-99-9	83.31
4-(Ethoxycarbonyl)phenylzinc iodide	131379-16-3	16.69

4. First-aid measures

General Advice	Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.
Eye Contact	Rinse 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.
Most important symptoms and effects	Causes burns by all exposure routes. Difficulty in breathing. 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. Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation
Notes to Physician	Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media	Dry sand. Carbon dioxide (CO ₂). Powder. Do not use water or foam. CO ₂ , 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	No information available
Explosion Limits	
Upper	No data available
Lower	No data 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. Zinc oxide.

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

Health
3

Flammability
3

Instability
2

Physical hazards
W

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 sources of ignition. Take precautionary measures against static discharges.

Environmental Precautions

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 Up

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. Acids. Acid chlorides. Oxidizing agent.

8. Exposure controls / personal protection

Exposure Guidelines

Component	ACGIH TLV	OSHA PEL	NIOSH	Mexico OEL (TWA)
Tetrahydrofuran	TWA: 50 ppm STEL: 100 ppm Skin	(Vacated) TWA: 200 ppm (Vacated) TWA: 590 mg/m ³ (Vacated) STEL: 250 ppm (Vacated) STEL: 735 mg/m ³ TWA: 200 ppm TWA: 590 mg/m ³	IDLH: 2000 ppm TWA: 200 ppm TWA: 590 mg/m ³ STEL: 250 ppm STEL: 735 mg/m ³	TWA: 200 ppm TWA: 590 mg/m ³ STEL: 250 ppm STEL: 735 mg/m ³

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.

Personal Protective Equipment

Eye/face Protection	Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.
Skin and body protection	Wear appropriate protective gloves and clothing to prevent skin exposure.
Respiratory Protection	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.
Recommended Filter type:	Organic gases and vapours filter. Type A. Brown. conforming to EN14387.
Hygiene Measures	Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

Physical State	Liquid
Appearance	Yellow - Brown - Black
Odor	No information available
Odor Threshold	No information available
pH	No information available
Melting Point/Range	No data available
Boiling Point/Range	66 °C / 150.8 °F
Flash Point	-17 °C / 1.4 °F
Evaporation Rate	No information available
Flammability (solid,gas)	Not applicable
Flammability or explosive limits	
Upper	No data available
Lower	No data available
Vapor Pressure	23 hPa @ 20 °C
Vapor Density	No information available
Specific Gravity	1.023 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 Formula	C9 H9 IO2 Zn
Molecular Weight	341.45

10. Stability and reactivity

Reactive Hazard	Yes
Stability	Air sensitive. Water reactive. May form precipitate.
Conditions to Avoid	Keep away from open flames, hot surfaces and sources of ignition.
Incompatible Materials	Acids, Acid chlorides, Oxidizing agent
Hazardous Decomposition Products	Carbon monoxide (CO), Carbon dioxide (CO ₂), Hydrogen iodide, Zinc oxide
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.

Dermal LD50

Based on ATE data, the classification criteria are not met. ATE > 2000 mg/kg.

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 Products

No information available

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

No information available

Sensitization

No information available

Carcinogenicity

Limited evidence of a carcinogenic effect. The table below indicates whether each agency 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
4-(Ethoxycarbonyl)phenylzinc iodide	131379-16-3	Not listed	Not listed	Not listed	Not listed	Not listed

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

A1 - Known Human Carcinogen

A2 - Suspected Human Carcinogen

A3 - Animal Carcinogen

ACGIH: (American Conference of Governmental Industrial Hygienists)

ACGIH: (American Conference of Governmental Industrial Hygienists)

Mutagenic Effects

No information available

Reproductive Effects

No information available.

Developmental Effects

No information available.

Teratogenicity

No information available.

STOT - single exposure

Respiratory system Central nervous system (CNS)

STOT - repeated exposure

None known

Aspiration hazard

No information available

Symptoms / effects, both acute and delayed

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: Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation

Endocrine Disruptor Information

Component	EU - Endocrine Disruptors Candidate List	EU - Endocrine Disruptors - Evaluated Substances	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 Pimephales promelas Leuciscus idus: LC50: 2820 mg/L/48h	Not listed	EC50 48 h 3485 mg/l EC50: >10000 mg/L/24h
-----------------	------------	--	------------	--

Persistence and Degradability based on information available. May persist

Bioaccumulation/ Accumulation No information available.

Mobility Will likely be mobile in the environment due to its volatility.

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 (4-(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

IATA

UN-No UN3399
Proper Shipping Name Organometallic substance, liquid, water-reactive, flammable
Hazard Class 4.3
Subsidiary Hazard Class 3
Packing Group II

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

United States of America Inventory

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	TSCA - EPA Regulatory Flags
Tetrahydrofuran	109-99-9	X	ACTIVE	-
4-(Ethoxycarbonyl)phenylzinc iodide	131379-16-3	-	-	-

Legend:

TSCA US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

X - Listed
 '-' - Not Listed

TSCA - Per 40 CFR 751, Regulation of Certain Chemical Substances & Mixtures, Under TSCA Section 6(h) (PBT)

Not applicable

TSCA 12(b) - Notices of Export

Component	CAS No	TSCA 12(b) - Notices of Export
Tetrahydrofuran	109-99-9	Section 4, 1 % de minimus concentration

International Inventories

Canada (DSL/NDL), Europe (EINECS/ELINCS/NLP), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), China (IECSC), Korea (KECL).

Component	CAS No	DSL	NDL	EINECS	PICCS	ENCS	ISHL	AICS	IECSC	KECL
Tetrahydrofuran	109-99-9	X	-	203-726-8	X	X	X	X	X	KE-33454
4-(Ethoxycarbonyl)phenylzinc iodide	131379-16-3	-	-	-	-	-	-	-	-	-

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

U.S. Federal Regulations
SARA 313

Section 313 of Title III of the Superfund Amendments and Reauthorization Act of 1986 (SARA). This product does not contain any chemicals which are subject to the reporting requirements of the Act and Title 40 of the Code of Federal Regulations, Part 372

SARA 311/312 Hazard Categories

Should this product meet EPCRA 311/312 Tier reporting criteria at 40 CFR 370, refer to Section 2 of this SDS for appropriate classifications.

CWA (Clean Water Act)

Not applicable

Clean Air Act

Not applicable

OSHA - Occupational Safety and Health Administration

Not applicable

CERCLA

This material, as supplied, contains one or more substances regulated as a hazardous substance under the Comprehensive Environmental Response Compensation and Liability Act (CERCLA) (40 CFR 302) or the Superfund Amendments and Reauthorization Act (SARA) (40 CFR 355).

Component	Hazardous Substances RQs	CERCLA Extremely Hazardous Substances RQs	SARA Reportable Quantity (RQ)
Tetrahydrofuran	1000 lb	-	1000 lb 454 kg

California Proposition 65

This product contains the following Proposition 65 chemicals.

Component	CAS No	California Prop. 65	Prop 65 NSRL	Category
Tetrahydrofuran	109-99-9	Carcinogen	-	Carcinogen

U.S. State Right-to-Know Regulations

Component	Massachusetts	New Jersey	Pennsylvania	Illinois	Rhode Island
Tetrahydrofuran	X	X	X	-	X

U.S. Department of Transportation

Reportable Quantity (RQ): Y
 DOT Marine Pollutant N
 DOT Severe Marine Pollutant N

U.S. Department of Homeland Security

This product does not contain any DHS chemicals.

Other International Regulations

Mexico - Grade No information available

Authorisation/Restrictions according to EU REACH

Component	CAS No	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization	REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
Tetrahydrofuran	109-99-9	-	Use restricted. See item 75. (see link for restriction details)	-
4-(Ethoxycarbonyl)phenylzinc iodide	131379-16-3	-	-	-

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
4-(Ethoxycarbonyl)phenylzinc iodide	131379-16-3	Not applicable	Not applicable	Not applicable	Not applicable

Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?

Not applicable

Other International Regulations

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
4-(Ethoxycarbonyl)phenylzinc iodide	131379-16-3	Not applicable	Not applicable	Not applicable	Not applicable

16. Other information**Prepared By**

Health, Safety and Environmental Department
 Email: chem.techinfo@thermofisher.com
 www.thermofisher.com

Revision Date	01-Apr-2024
Print Date	01-Apr-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