

SAFETY DATA SHEET

Revision Date 01-Apr-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

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

Hazard(s) identification

Classification

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

Flammable liquids

Acute oral toxicity

Skin Corrosion/Irritation

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 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 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

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

Wash contaminated clothing before reuse

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

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

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
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.

Most important symptoms and

effects

Causes burns by all exposure routes. Difficulty in breathing. 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 Treat symptomatically

Notes to Physician

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

No information available

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. 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

Health Flammability Instability Physical hazards
3 3 2 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. 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.

Environmental Precautions

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.

Up

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

Wear appropriate protective eyeglasses or chemical safety goggles as described by **Eye/face Protection**

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: low boiling organic solvent. Type AX. Brown. conforming to EN371. or. 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

AppearanceYellow - Brown - BlackOdorNo information availableOdor ThresholdNo information available

pH No information available

Melting Point/RangeNo data availableBoiling Point/RangeNo information availableFlash Point-17 °C / 1.4 °FEvaporation RateNo information available

Flammability (solid,gas)

Not applicable

Flammability (solid,gas)
Flammability or explosive limits

UpperNo data availableLowerNo data availableVapor PressureNo information available

Vapor Pressure
No information available
Specific Gravity
No information available
0.991 g/cm3

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.

Dermal LD50Based 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

No information available Irritation 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
3-(Ethoxycarbonyl)phe nylzinc iodide	282727-18-8	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

ACGIH: (American Conference of Governmental Industrial

Hygienists)

A1 - Known Human Carcinogen A2 - Suspected Human Carcinogen

A3 - Animal Carcinogen

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)

None known STOT - repeated exposure

No information available **Aspiration hazard**

delayed

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	EU - Endocrine Disrupters	EU - Endocrine Disruptors -	Japan - Endocrine Disruptor
	Candidate List	Evaluated Substances	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 ||

TDG

UN-No UN3399

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

Hazard Class 4.3
Subsidiary Hazard Class
Packing Group

<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

United States of America Inventory

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	TSCA - EPA Regulatory Flags
Tetrahydrofuran	109-99-9	X	ACTIVE	-
3-(Ethoxycarbonyl)phenylzinc iodide	282727-18-8	-	-	-

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

Component	CAS No	DSL	NDSL	EINECS	PICCS	ENCS	ISHL	AICS	IECSC	KECL
Tetrahydrofuran	109-99-9	Χ	-	203-726-8	Χ	Χ	Χ	Χ	Χ	KE-33454
3-(Ethoxycarbonyl)phenylzinc iodide	282727-18-8	-	1	-	ı	-		Ī	Ī	1

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

January and Januar

Not applicable

Health Administration

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

This product does not contain any DHS chemicals.

Security

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 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)	-
3-(Ethoxycarbonyl)phenylzinc iodide	282727-18-8	-	-	-

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

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
3-(Ethoxycarbonyl)phenylzinc iodide	282727-18-8	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

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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