

ALFAAA15123

2-Phenylethyl isothiocyanate

SECTION 1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

产品说明:
Product Description: 2-苯基乙基 异硫氰酸酯
2-Phenylethyl isothiocyanate

Cat No. : A15123
Synonyms 2-Isothiocyanatoethylbenzene
CAS No 2257-09-2
Molecular Formula C9 H9 N S

Supplier Avocado Research Chemicals Ltd.
(Part of Thermo Fisher Scientific)
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United Kingdom
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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

E-mail address begel.sdsdesk@thermofisher.com

Recommended Use Laboratory chemicals.
Uses advised against No Information available

SECTION 2. HAZARD IDENTIFICATION

Physical State
Liquid

Appearance
Light yellow

Odor
Odorless

Emergency Overview

Harmful if swallowed. Harmful in contact with skin. Causes skin irritation. Causes serious eye irritation. Harmful if inhaled. May cause allergy or asthma symptoms or breathing difficulties if inhaled. May cause respiratory irritation. Moisture sensitive.
Lachrymator (substance which increases the flow of tears).

Classification of the substance or mixture

Acute Oral Toxicity	Category 4
Acute Dermal Toxicity	Category 4
Acute Inhalation Toxicity - Vapors	Category 4
Skin Corrosion/Irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 2
Respiratory Sensitization	Category 1
Specific target organ toxicity - (single exposure)	Category 3

Label Elements

2-Phenylethyl isothiocyanate



Signal Word

Danger

Hazard Statements

H315 - Causes skin irritation

H319 - Causes serious eye irritation

H334 - May cause allergy or asthma symptoms or breathing difficulties if inhaled

H335 - May cause respiratory irritation

H302 + H312 + H332 - Harmful if swallowed, in contact with skin or if inhaled

Precautionary Statements

Prevention

P261 - Avoid breathing dust/fume/gas/mist/vapors/spray

P264 - Wash face, hands and any exposed 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

P284 - In case of inadequate ventilation wear respiratory protection

Response

P302 + P352 - IF ON SKIN: Wash with plenty of soap and water

P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing

P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing

P312 - Call a POISON CENTER or doctor if you feel unwell

P330 - Rinse mouth

P342 + P311 - If experiencing respiratory symptoms: Call a POISON CENTER or doctor

P362 + P364 - Take off contaminated clothing and wash it before reuse

Storage

P403 + P233 - Store in a well-ventilated place. Keep container tightly closed

Disposal

P501 - Dispose of contents/ container to an approved waste disposal plant

Physical and Chemical Hazards

None identified.

Health Hazards

Harmful if swallowed. Harmful in contact with skin. Causes skin irritation. Causes serious eye irritation. Harmful if inhaled. May cause allergy or asthma symptoms or breathing difficulties if inhaled. May cause respiratory irritation. Lachrymator (substance which increases the flow of tears).

Environmental hazards

Contains no substances known to be hazardous to the environment or not degradable in waste water treatment plants. Is not likely mobile in the environment due its low water solubility. Will likely be mobile in the environment due to its volatility. The product is insoluble and sinks in water. The product contains volatile organic compounds (VOC) which will evaporate easily from all surfaces. Spillage unlikely to penetrate soil.

Other Hazards

Lachrymator (substance which increases the flow of tears)

This product does not contain any known or suspected endocrine disruptors.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Component	CAS No	Weight %
Benzene, (2-isothiocyanatoethyl)-	2257-09-2	>95

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SECTION 4. FIRST AID MEASURES

General Advice

If symptoms persist, call a physician.

Eye Contact

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.

Skin Contact

Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, call a physician.

Inhalation

Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur.

Ingestion

Clean mouth with water and drink afterwards plenty of water.

Most important symptoms and effects

None reasonably foreseeable. May cause allergy or asthma symptoms or breathing difficulties if inhaled. Symptoms of allergic reaction may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing

Self-Protection of the First Aider

Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.

Notes to Physician

Treat symptomatically.

SECTION 5. FIRE-FIGHTING MEASURES

Suitable Extinguishing Media

CO₂, dry chemical, dry sand, alcohol-resistant foam.

Extinguishing media which must not be used for safety reasons

No information available.

Specific Hazards Arising from the Chemical

Thermal decomposition can lead to release of irritating gases and vapors.

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.

SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal Precautions

Use personal protective equipment as required. Ensure adequate ventilation.

Environmental Precautions

Should not be released into the environment.

Methods for Containment and Clean Up

Soak up with inert absorbent material. Keep in suitable, closed containers for disposal.

Refer to protective measures listed in Sections 8 and 13.

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SECTION 7. HANDLING AND STORAGE

Handling

Ensure adequate ventilation. Wear personal protective equipment/face protection. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation.

Storage

Keep in a dry, cool and well-ventilated place. Keep container tightly closed. Store under an inert atmosphere.

Specific Use(s)

Use in laboratories

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Control Parameters**Monitoring methods**

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents. MDHS70 General methods for sampling airborne gases and vapours MDHS 96 Volatile organic compounds in air - Laboratory method using pumped solid sorbent tubes, solvent desorption and gas chromatography

Exposure Controls**Engineering Measures**

Ensure adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation location. 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 (European standard - EN 166)

Hand Protection Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Natural rubber	See manufacturers	-	EN 374	(minimum requirement)
Nitrile rubber	recommendations			
Neoprene				
PVC				

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, 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.

Remove gloves with care avoiding skin contamination.

Skin and body protection Wear appropriate protective gloves and clothing to prevent skin exposure

Respiratory Protection When workers are facing concentrations above the exposure limit they must use appropriate certified respirators.
To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

Large scale/emergency use Use a NIOSH/MSHA or European Standard EN 136 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

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Small scale/Laboratory use

Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

Recommended half mask:- Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 141

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

Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice.

Environmental exposure controls

No information available.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance	Light yellow	
Physical State	Liquid	
Odor	Odorless	
Odor Threshold	No data available	
pH	Not applicable	
Melting Point/Range	No data available	
Softening Point	No data available	
Boiling Point/Range	113 °C / 235.4 °F	@ 1 mmHg
Flash Point	100 °C / 212 °F	Method - No information available
Evaporation Rate	No data available	
Flammability (solid,gas)	Not applicable	Liquid
Explosion Limits	No data available	
Vapor Pressure	No data available	
Vapor Density	5.63	(Air = 1.0)
Specific Gravity / Density	1.100	
Bulk Density	Not applicable	Liquid
Water Solubility	Insoluble	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Component	log Pow	
Benzene, (2-isothiocyanatoethyl)-	3.47	
Autoignition Temperature	No data available	
Decomposition Temperature	No data available	
Viscosity	No data available	
Explosive Properties	No information available	
Oxidizing Properties	No information available	
Molecular Formula	C9 H9 N S	
Molecular Weight	163.24	

SECTION 10. STABILITY AND REACTIVITY

Stability	Stable under recommended storage conditions. Moisture sensitive.
Hazardous Reactions	None under normal processing.
Hazardous Polymerization	Hazardous polymerization does not occur.
Conditions to Avoid	Incompatible products. Excess heat. Exposure to moist air or water.
Materials to avoid	Strong oxidizing agents.

Hazardous Decomposition Products Carbon monoxide (CO). Carbon dioxide (CO₂). Hydrogen cyanide (hydrocyanic acid). Nitrogen oxides (NO_x). Sulfur oxides. Thermal decomposition can lead to release of

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irritating gases and vapors.

SECTION 11. TOXICOLOGICAL INFORMATION

Product Information

(a) acute toxicity;

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Benzene, (2-isothiocyanatoethyl)-	700 mg/kg (Mouse)		

(b) skin corrosion/irritation; Category 2

(c) serious eye damage/irritation; Category 2

(d) respiratory or skin sensitization;

Respiratory	Category 1
Skin	No data available

(e) germ cell mutagenicity; No data available

(f) carcinogenicity; No data available

There are no known carcinogenic chemicals in this product

(g) reproductive toxicity; No data available

(h) STOT-single exposure; Category 3

Results / Target organs	Respiratory system
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(i) STOT-repeated exposure; No data available

Target Organs	None known.
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(j) aspiration hazard; No data available

Other Adverse Effects The toxicological properties have not been fully investigated.

Symptoms / effects, both acute and delayed Symptoms of allergic reaction may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity effects Do not empty into drains. .

Persistence and Degradability

Persistence	Persistence is unlikely.
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Bioaccumulative Potential Bioaccumulation is unlikely

Component	log Pow	Bioconcentration factor (BCF)
Benzene, (2-isothiocyanatoethyl)-	3.47	No data available

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Mobility in soil

The product is insoluble and sinks in water The product contains volatile organic compounds (VOC) which will evaporate easily from all surfaces Spillage unlikely to penetrate soil Is not likely mobile in the environment due its low water solubility Will likely be mobile in the environment due to its volatility

**Endocrine Disruptor Information
Persistent Organic Pollutant
Ozone Depletion Potential**

This product does not contain any known or suspected endocrine disruptors
This product does not contain any known or suspected substance
This product does not contain any known or suspected substance

SECTION 13. DISPOSAL CONSIDERATIONS**Waste from Residues/Unused Products**

Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.

Contaminated Packaging

Dispose of this container to hazardous or special waste collection point.

Other Information

Waste codes should be assigned by the user based on the application for which the product was used. Do not empty into drains.

SECTION 14. TRANSPORT INFORMATION**Road and Rail Transport**

UN-No UN2206
Proper Shipping Name ISOCYANATES, TOXIC, N.O.S.
Technical Shipping Name Phenylethyl isothiocyanate
Hazard Class 6.1
Packing Group III

IMDG/IMO

UN-No UN2206
Proper Shipping Name ISOCYANATES, TOXIC, N.O.S.
Technical Shipping Name Phenylethyl isothiocyanate
Hazard Class 6.1
Packing Group III

IATA

UN-No UN2206
Proper Shipping Name ISOCYANATE SOLUTION, TOXIC, N.O.S.
Technical Shipping Name Phenylethyl isothiocyanate
Hazard Class 6.1
Packing Group III

Special Precautions for User

No special precautions required

SECTION 15. REGULATORY INFORMATION**International Inventories**

China, X = listed, Australia, U.S.A. (TSCA), Canada (DSL/NDSL), Europe (EINECS/ELINCS/NLP), Australia (AICS), Korea (KECL), China (IECSC), Japan (ENCS), Philippines (PICCS), Taiwan (TCSI), Japan (ISHL), New Zealand (NZIoC), Japan (ISHL).

Component	The Inventory of Hazardous Chemicals (2015)	List of dangerous goods GB 12268 - 2012	TCSI	IECSC	EINECS	TSCA	DSL	PICCS	ENCS	ISHL	AICS	KECL

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	Edition)											
Benzene, (2-isothiocyanatoethyl) -	-	-	X	X	218-855-5	X	X	X	-		X	-

National Regulations

SECTION 16. OTHER INFORMATION

Prepared By Health, Safety and Environmental Department
Creation Date 03-Oct-2011
Revision Date 22-Apr-2024
Revision Summary New emergency telephone response service provider.

Training Advice

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

Legend

CAS - Chemical Abstracts Service

EINECS/ELINCS - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

PICCS - Philippines Inventory of Chemicals and Chemical Substances

IECSC - Chinese Inventory of Existing Chemical Substances

KECL - Korean Existing and Evaluated Chemical Substances

TSCA - United States Toxic Substances Control Act Section 8(b) Inventory

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

ENCS - Japanese Existing and New Chemical Substances

AICS - Australian Inventory of Chemical Substances

NZIoC - New Zealand Inventory of Chemicals

WEL - Workplace Exposure Limit

ACGIH - American Conference of Governmental Industrial Hygienists

DNEL - Derived No Effect Level

RPE - Respiratory Protective Equipment

LC50 - Lethal Concentration 50%

NOEC - No Observed Effect Concentration

PBT - Persistent, Bioaccumulative, Toxic

TWA - Time Weighted Average

IARC - International Agency for Research on Cancer

PNEC - Predicted No Effect Concentration

LD50 - Lethal Dose 50%

EC50 - Effective Concentration 50%

POW - Partition coefficient Octanol:Water

vPvB - very Persistent, very Bioaccumulative

ICAO/IATA - International Civil Aviation Organization/International Air Transport Association

ADR - European Agreement Concerning the International Carriage of Dangerous Goods by Road

OECD - Organisation for Economic Co-operation and Development

BCF - Bioconcentration factor

IMO/IMDG - International Maritime Organization/International Maritime Dangerous Goods Code

MARPOL - International Convention for the Prevention of Pollution from Ships

ATE - Acute Toxicity Estimate

VOC - (Volatile Organic Compound)

Key literature references and sources for data

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

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

SAFETY DATA SHEET
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End of Safety Data Sheet