

SAFETY DATA SHEET

Creation Date 03-Oct-2011

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Revision Number 4

1. Identification

Product Name 2-Phenylethyl isothiocyanate

Cat No. : A15123

CAS No 2257-09-2
Synonyms 2-Isothiocyanatoethylbenzene

Recommended Use Laboratory chemicals.
Uses advised against Food, drug, pesticide or biocidal product use.

Details of the supplier of the safety data sheet

Company

Alfa Aesar
Thermo Fisher Scientific Chemicals, Inc.
30 Bond Street
Ward Hill, MA 01835-8099
Tel: 800-343-0660
Fax: 800-322-4757
Email: tech@alfa.com
www.alfa.com

Emergency Telephone Number During normal business hours (Monday-Friday, 8am-7pm EST), call (800) 343-0660.
After normal business hours, call Carechem 24 at (866) 928-0789.

2. Hazard(s) identification

Classification

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

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
Target Organs - Respiratory system.	

Label Elements

Signal Word

Danger

Hazard Statements

Causes skin irritation

Causes serious eye irritation

May cause allergy or asthma symptoms or breathing difficulties if inhaled

May cause respiratory irritation

Harmful if swallowed, in contact with skin or if inhaled

**Precautionary Statements****Prevention**

Wash face, hands and any exposed skin thoroughly after handling

Do not eat, drink or smoke when using this product

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

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

Use only outdoors or in a well-ventilated area

In case of inadequate ventilation wear respiratory protection

Inhalation

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

If experiencing respiratory symptoms: Call a POISON CENTER or doctor/physician

Skin

IF ON SKIN: Wash with plenty of soap and water

Call a POISON CENTER or doctor/physician if you feel unwell

If skin irritation occurs: Get medical advice/attention

Take off contaminated clothing and wash before reuse

Eyes

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

If eye irritation persists: Get medical advice/attention

Ingestion

IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell

Rinse mouth

Storage

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

Store locked up

Disposal

Dispose of contents/container to an approved waste disposal plant

Hazards not otherwise classified (HNOC)

None identified

3. Composition/Information on Ingredients

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

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
Notes to Physician	Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media	CO ₂ , dry chemical, dry sand, alcohol-resistant foam.
Unsuitable Extinguishing Media	No information available
Flash Point	100 °C / 212 °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.

Hazardous Combustion Products

Carbon monoxide (CO). Carbon dioxide (CO₂). Hydrogen cyanide (hydrocyanic acid). Nitrogen oxides (NO_x). Sulfur oxides. 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.

NFPA

Health
2

Flammability
1

Instability
0

Physical hazards
N/A

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.

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.
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Storage. Keep in a dry, cool and well-ventilated place. Keep container tightly closed. Store under an inert atmosphere. Incompatible Materials. Strong oxidizing agents.

8. Exposure controls / personal protection

Exposure Guidelines This product does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies.

Engineering Measures Ensure adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation location.

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.

Hygiene Measures Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

Physical State	Liquid
Appearance	Light yellow
Odor	Odorless
Odor Threshold	No information available
pH	Not applicable
Melting Point/Range	No data available
Boiling Point/Range	113 °C / 235.4 °F @ 1 mmHg
Flash Point	100 °C / 212 °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	No information available
Vapor Density	5.63
Specific Gravity	1.100
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 N S
Molecular Weight	163.24

10. Stability and reactivity

Reactive Hazard None known, based on information available

Stability Stable under recommended storage conditions. Moisture sensitive.

Conditions to Avoid	Incompatible products. Excess heat. Exposure to moist air or water.
Incompatible Materials	Strong oxidizing agents
Hazardous Decomposition Products	Carbon monoxide (CO), Carbon dioxide (CO ₂), Hydrogen cyanide (hydrocyanic acid), Nitrogen oxides (NO _x), Sulfur oxides, Thermal decomposition can lead to release of irritating gases and vapors
Hazardous Polymerization	Hazardous polymerization does not occur.
Hazardous Reactions	None under normal processing.

11. Toxicological information

Acute Toxicity

Product Information Component Information

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Benzene, (2-isothiocyanatoethyl)-	700 mg/kg (Mouse)	Not listed	Not listed

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	The table below indicates whether each agency has listed any ingredient as a carcinogen.

Component	CAS No	IARC	NTP	ACGIH	OSHA	Mexico
Benzene, (2-isothiocyanatoethyl)-	2257-09-2	Not listed	Not listed	Not listed	Not listed	Not listed

Mutagenic Effects	No information available
Reproductive Effects	No information available.
Developmental Effects	No information available.
Teratogenicity	No information available.
STOT - single exposure	Respiratory system
STOT - repeated exposure	None known
Aspiration hazard	No information available
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
Endocrine Disruptor Information	No information available
Other Adverse Effects	The toxicological properties have not been fully investigated.

12. Ecological information

Ecotoxicity

Do not empty into drains. .

Persistence and Degradability	Persistence is unlikely
Bioaccumulation/ Accumulation	No information available.

Mobility Is not likely mobile in the environment due its low water solubility. Will likely be mobile in the environment due to its volatility.

Component	log Pow
Benzene, (2-isothiocyanatoethyl)-	3.47

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.

14. Transport information

DOT

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

TDG

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

IATA

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

IMDG/IMO

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

15. Regulatory information

United States of America Inventory

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	TSCA - EPA Regulatory Flags
Benzene, (2-isothiocyanatoethyl)-	2257-09-2	X	ACTIVE	-

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

Not applicable

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	CAS No	DSL	NDSL	EINECS	PICCS	ENCS	ISHL	AICS	IECSC	KECL
Benzene, (2-isothiocyanatoethyl)-	2257-09-2	X	-	218-855-5	X	-		X	X	-

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

U.S. Federal Regulations

SARA 313	Not applicable
SARA 311/312 Hazard Categories	See section 2 for more information
CWA (Clean Water Act)	Not applicable
Clean Air Act	Not applicable
OSHA - Occupational Safety and Health Administration	Not applicable
CERCLA	Not applicable
California Proposition 65	This product does not contain any Proposition 65 chemicals.
U.S. State Right-to-Know Regulations	Not applicable

U.S. Department of Transportation

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

U.S. Department of Homeland Security	This product does not contain any DHS chemicals.
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Other International Regulations

Mexico - Grade	No information available
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Authorisation/Restrictions according to EU REACH	Not applicable
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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)
Benzene, (2-isothiocyanatoethyl)-	2257-09-2	-	-	-

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)
Benzene, (2-isothiocyanatoethyl)-	2257-09-2	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)
Benzene, (2-isothiocyanatoethyl)-	2257-09-2	Not applicable	Not applicable	Not applicable	Not applicable

16. Other information

Prepared By	Health, Safety and Environmental Department Email: tech@alfa.com www.alfa.com
Creation Date	03-Oct-2011
Revision Date	12-Apr-2022
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Revision Summary	SDS authoring systems update, replaces ChemGes SDS No. 2257-09-2.

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