

Chemical Safety Data Sheet MSDS / SDS

Phenethyl isothiocyanate

Revision Date:2025-02-01 Revision Number:1

SECTION 1: Identification of the substance/mixture and of the company/undertaking

Product identifier

Product name : Phenethyl isothiocyanate
CBnumber : CB2736659
CAS : 2257-09-2
EINECS Number : 218-855-5
Synonyms : phenethyl isothiocyanate, Benzene, (2-isothiocyanatoethyl)-

Relevant identified uses of the substance or mixture and uses advised against

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.
Uses advised against : none

Company Identification

Company : Chemicalbook
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone : 400-158-6606

SECTION 2: Hazards identification

GHS Label elements, including precautionary statements

Symbol(GHS)



Signal word

Danger

Precautionary statements

P342+P311 IF experiencing respiratory symptoms: call a POISON CENTER or doctor/physician.

P405 Store locked up.

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

P303+P361+P353 IF ON SKIN (or hair): Remove/Take off Immediately all contaminated clothing. Rinse SKIN with water/shower.

P301+P330+P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

P284 Wear respiratory protection.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

Hazard statements

H302 Harmful if swallowed
H312 Harmful in contact with skin
H314 Causes severe skin burns and eye damage
H315 Causes skin irritation
H317 May cause an allergic skin reaction
H335 May cause respiratory irritation
H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled
H332 Harmful if inhaled
H331 Toxic if inhaled
H319 Causes serious eye irritation
H318 Causes serious eye damage

SECTION 3: Composition/information on ingredients

Substance

Product name	: Phenethyl isothiocyanate
Synonyms	: phenethyl isothiocyanate, Benzene, (2-isothiocyanatoethyl)-
CAS	: 2257-09-2
EC number	: 218-855-5
MF	: C9H9NS
MW	: 163.24

SECTION 4: First aid measures

Description of first aid measures

General advice

Consult a physician. Show this material safety data sheet to the doctor in attendance.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

Extinguishing media

Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

Special hazards arising from the substance or mixture

Carbon oxides, Nitrogen oxides (NO_x), Sulfur oxides

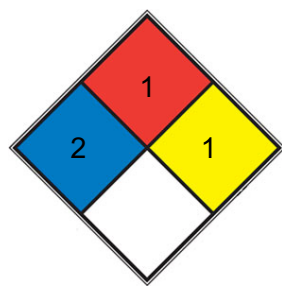
Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

Further information

No data available

NFPA 704



HEALTH 2 Intense or continued but not chronic exposure could cause temporary incapacitation or possible residual injury (e.g. [diethyl ether](#), ammonium phosphate, iodine)

FIRE 1 Materials that require considerable preheating, under all ambient temperature conditions, before ignition and combustion can occur. Includes some finely divided suspended solids that do not require heating before ignition can occur. Flash point at or above 93.3 °C (200 °F). (e.g. [mineral oil](#), ammonia)

REACT 1 Normally stable, but can become unstable at elevated temperatures and pressures (e.g. [propene](#))

SPEC.

HAZ.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas.

For personal protection see section 8.

Environmental precautions

Do not let product enter drains.

Methods and materials for containment and cleaning up

Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapor or mist. For precautions see section 2.2.

Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage. Store in cool place.

Recommended storage temperature 2 - 8 °C Moisture sensitive.

Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

control parameter

Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

Exposure controls

Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye/face protection

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

Body Protection

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full- face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and

components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

Do not let product enter drains.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Appearance	colorless clear, liquid
Odour	No data available
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	143~145°C
Initial boiling point and boiling range	139 - 140 °C at 15 hPa - lit.
Flash point	113 °C - closed cup
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	No data available
Vapour pressure	No data available
Vapour density	No data available
Relative density	1,094 g/cm ³ at 25 °C
Water solubility	No data available
Partition coefficient: n-octanol/water	No data available
Autoignition temperature	No data available
Decomposition temperature	No data available
Viscosity	No data available
Explosive properties	No data available
Oxidizing properties	No data available

Other safety information

No data available

SECTION 10: Stability and reactivity

Reactivity

No data available

Chemical stability

Stable under recommended storage conditions.

Possibility of hazardous reactions

No data available

Conditions to avoid

Heat. Avoid moisture.

Incompatible materials

Water, Alcohols, Strong bases, Amines, acids, Strong oxidizing agents

Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NOx), Sulfur oxides

Other decomposition products - No data available In the event of fire: see section 5

SECTION 11: Toxicological information

Information on toxicological effects

Acute toxicity

LD50 Oral - Mouse - 700 mg/kg

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

Hamster ovary

Cytogenetic analysis Hamster

ovary

Sister chromatid exchange

Mammal Cytogenetic analysis

Mammal

Other mutation test systems

Carcinogenicity

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

Inhalation - May cause respiratory irritation.

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

Additional Information

RTECS: NX9115000

Cough, Shortness of breath, Headache, Nausea, Vomiting, Repeated exposure may cause asthma., prolonged or repeated exposure can cause:, Lung irritation

Toxicity

LD50 in mice (mg/kg): 700 orally; 150 s.c.; 50 i.v. (Lichtenstein)

SECTION 12: Ecological information

Toxicity

No data available

Toxicity to daphnia and other aquatic invertebrates

LC50 - Daphnia magna (Water flea) - 0,13 mg/l - 48 h

Persistence and degradability

No data available

Bioaccumulative potential

No data available

Mobility in soil

No data available

Results of PBT and vPvB assessment

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

Other adverse effects

No data available

SECTION 13: Disposal considerations

Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Waste material must be disposed of in accordance with the Directive on waste 2008/98/EC as well as other national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

UN number

ADR/RID: 2206 IMDG: 2206 IATA: 2206

UN proper shipping name

ADR/RID: ISOCYANATE SOLUTION, TOXIC, N.O.S. (Phenethyl isothiocyanate) IMDG: ISOCYANATE SOLUTION, TOXIC, N.O.S. (Phenethyl isothiocyanate) IATA: Isocyanate solution, toxic, n.o.s. (Phenethyl isothiocyanate)

Transport hazard class(es)

ADR/RID: 6.1 IMDG: 6.1 IATA: 6.1

Packaging group

ADR/RID: III IMDG: III IATA: III

Environmental hazards

ADR/RID: no IMDG Marine pollutant: no IATA: no

Special precautions for user

No data available

SECTION 15: Regulatory information

Safety, health and environmental regulations/legislation specific for the substance or mixture**Regulations on the Safety Management of Hazardous Chemicals**

China Catalog of Hazardous chemicals 2015:Not Listed. website: <https://www.mem.gov.cn/>

Measures for Environmental Management of New Chemical Substances

Korea Existing Chemicals List (KECL):Not Listed. website: <http://ncis.nier.go.kr>

Vietnam National Chemical Inventory:Listed. website: <https://chemicaldata.gov.vn/>

United States Toxic Substances Control Act (TSCA) Inventory:Listed. website: <https://www.epa.gov/>

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Listed. website: <https://emb.gov.ph/>

New Zealand Inventory of Chemicals (NZIoC):Listed. website: <https://www.epa.govt.nz/>

European Inventory of Existing Commercial Chemical Substances (EINECS):Listed. website: <https://echa.europa.eu/>

EC Inventory:Listed.

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Listed. website: <https://www.mee.gov.cn/>

SECTION 16: Other information

Abbreviations and acronyms

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

CAS: Chemical Abstracts Service

EC50: Effective Concentration 50%

IATA: International Air Transportation Association

IMDG: International Maritime Dangerous Goods

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

STEL: Short term exposure limit

TWA: Time Weighted Average

References

- 【1】 CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>
- 【2】 ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>
- 【3】 ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>
- 【4】 eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:
http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en
- 【5】 ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>
- 【6】 Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>
- 【7】 HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>
- 【8】 IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>
- 【9】 IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>
- 【10】 Sigma-Aldrich, website: <https://www.sigmaaldrich.com/>

Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.