Material Safety Data Sheet

Version 4.0
Revision Date 03/14/2010
Print Date 09/20/2010

1. PRODUCT AND COMPANY IDENTIFICATION

Product name	:	2-Phenylethyl isothiocyanate
Product Number	:	W401404
Brand	:	Aldrich
Company	:	Sigma-Aldrich 3050 Spruce Street SAINT LOUIS MO 63103 USA
Telephone	:	+18003255832
Fax	:	+18003255052
Emergency Phone #	:	(314) 776-6555

2. HAZARDS IDENTIFICATION

Emergency Overview

OSHA Hazards
Harmful by ingestion., Irritant

Other hazards which do not result in classification
Lachrymator.

GHS Label elements, including precautionary statements

Pictogram

Signal word Danger

Hazard statement(s)

H302 + H312	Harmful if swallowed or in contact with skin.
H315	Causes skin irritation.
H317	May cause an allergic skin reaction.
H319	Causes serious eye irritation.
H332	Harmful if inhaled.
H334	May cause allergy or asthma symptoms or breathing difficulties if inhaled.
H335	May cause respiratory irritation.

Precautionary statement(s)

P261	Avoid breathing dust/fume/gas/mist/vapours/spray.
P280	Wear protective gloves/protective clothing.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P342 + P311	If experiencing respiratory symptoms: Call a POISON CENTER or doctor/physician.

HMIS Classification

Health hazard:	2
Flammability:	1
Physical hazards:	0

NFPA Rating

Health hazard:	2
Fire:	1
Reactivity Hazard:	0

Potential Health Effects

Inhalation	May be harmful if inhaled. Causes respiratory tract irritation.
Skin	May be harmful if absorbed through skin. Causes skin irritation.
Eyes	Causes eye irritation.
Ingestion	Harmful if swallowed.

3. COMPOSITION/INFORMATION ON INGREDIENTS

Synonyms : Phenethyl isothiocyanate
2-Phenylethyl isothiocyanate

Formula : C_9H_9NS

Molecular Weight : 163.24 g/mol

CAS-No.	EC-No.	Index-No.	Concentration
Phenethyl isothiocyanate			
2257-09-2	218-855-5	-	-

4. FIRST AID MEASURES

General advice
Consult a physician. Show this safety data sheet to the doctor in attendance.Move out of dangerous area.

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.

5. FIRE-FIGHTING MEASURES

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

Special protective equipment for fire-fighters
Wear self contained breathing apparatus for fire fighting if necessary.

6. ACCIDENTAL RELEASE MEASURES

Personal precautions
Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation.

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.

7. HANDLING AND STORAGE

Precautions for safe handling
Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.
Normal measures for preventive fire protection.

Conditions for safe storage
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.

Recommended storage temperature: 2 - 8 °C

Moisture sensitive.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Contains no substances with occupational exposure limit values.

Personal protective equipment

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).

Hand protection
Handle with gloves.

Eye protection
Face shield and safety glasses

Skin and body protection
Choose body protection according to the amount and concentration of the dangerous substance at the work place.

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

9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance

Form	clear, liquid
Colour	colourless

Safety data

pH	no data available
Melting point	no data available
Boiling point	139 - 140 °C (282 - 284 °F) at 15 hPa (11 mmHg) - lit.
Flash point	113 °C (235 °F) - closed cup
Ignition temperature	no data available
Lower explosion limit	no data available
Upper explosion limit	no data available
Density	1.094 g/cm3 at 25 °C (77 °F)
Water solubility	no data available

10. STABILITY AND REACTIVITY

Chemical stability
Stable under recommended storage conditions.

Conditions to avoid
Heat. Avoid moisture.

Materials to avoid
Water, Alcohols, Strong bases, Amines, acids, Strong oxidizing agents

Hazardous decomposition products
Hazardous decomposition products formed under fire conditions. - Carbon oxides, nitrogen oxides (NOx), Sulphur oxides

11. TOXICOLOGICAL INFORMATION

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

May cause allergic respiratory and skin reactions

Germ cell mutagenicity

Genotoxicity in vitro - Hamster - ovary
Cytogenetic analysis

Genotoxicity in vitro - Hamster - ovary
Sister chromatid exchange

Genotoxicity in vivo - Mammal - Skin
Cytogenetic analysis

Genotoxicity in vivo - Mammal - Skin
Other mutation test systems

Carcinogenicity

IARC:	No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.
ACGIH:	No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.
NTP:	No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.
OSHA:	No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

Reproductive toxicity
no data available

Specific target organ toxicity - single exposure (GHS)
Inhalation - May cause respiratory irritation.

Specific target organ toxicity - repeated exposure (GHS)
no data available

Aspiration hazard
no data available

Potential health effects

Inhalation	May be harmful if inhaled. Causes respiratory tract irritation.
Ingestion	Harmful if swallowed.
Skin	May be harmful if absorbed through skin. Causes skin irritation.
Eyes	Causes eye irritation.

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

Additional Information
RTECS: NX9115000

12. ECOLOGICAL INFORMATION

Toxicity

Toxicity to daphnia	LC50 - Daphnia magna (Water flea) - 0.13 mg/l - 48 h

and other aquatic
invertebrates.

Persistence and degradability
no data available

Bioaccumulative potential
no data available

Mobility in soil
no data available

PBT and vPvB assessment
no data available

Other adverse effects

no data available

13. DISPOSAL CONSIDERATIONS

Product
Observe all federal, state, and local environmental regulations. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging
Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)
UN-Number: 2206 Class: 6.1 Packing group: III
Proper shipping name: Isocyanate solutions, toxic, n.o.s.
Marine pollutant: No
Poison Inhalation Hazard: No

IMDG
UN-Number: 2206 Class: 6.1 Packing group: III EMS-No: F-A, S-A
Proper shipping name: ISOCYANATE SOLUTION, TOXIC, N.O.S.
Marine pollutant: No

IATA
UN-Number: 2206 Class: 6.1 Packing group: III
Proper shipping name: Isocyanate solution, toxic, n.o.s.

15. REGULATORY INFORMATION

OSHA Hazards
Harmful by ingestion., Irritant

DSL Status
All components of this product are on the Canadian DSL list.

SARA 302 Components
SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components
SARA 313: This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards
Acute Health Hazard

Massachusetts Right To Know Components
No components are subject to the Massachusetts Right to Know Act.

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Phenethyl isothiocyanate	2257-09-2	

New Jersey Right To Know Components

	CAS-No.	Revision Date
Phenethyl isothiocyanate	2257-09-2	

California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION

Further information

Copyright 2010 Sigma-Aldrich Co. License granted to make unlimited paper copies for internal use only.
The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Co., shall not be held liable for any damage resulting from handling or from contact with the above product. See reverse side of invoice or packing slip for additional terms and conditions of sale.