1. PRODUCT AND COMPANY IDENTIFICATION

Product name: Phenyl isothiocyanate
Product Number: 139742
Brand: Aldrich
Supplier: Sigma-Aldrich Corporation
3050 Spruce Street
SAINT LOUIS MO  63103
USA
Telephone: +1 800-325-5832
Fax: +1 800-325-5052
Emergency Phone #: (314) 776-6555
Preparation Information: Sigma-Aldrich Corporation
Product Safety - Americas Region
1-800-521-8956

2. HAZARDS IDENTIFICATION

Emergency Overview

OSHA Hazards
Combustible Liquid, Target Organ Effect, Toxic by ingestion, Corrosive

Target Organs
Kidney, Bladder

Other hazards which do not result in classification
Lachrymator.

GHS Classification
Flammable liquids (Category 4)
Acute toxicity, Oral (Category 3)
Skin corrosion (Category 1B)
Serious eye damage (Category 1)
Respiratory sensitization (Category 1)
Skin sensitization (Category 1)
Acute aquatic toxicity (Category 2)

GHS Label elements, including precautionary statements

Pictogram

Signal word Danger

Hazard statement(s)
H227 Combustible liquid
H301 Toxic if swallowed.
H314 Causes severe skin burns and eye damage.
H317 May cause an allergic skin reaction.
H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled.
H401 Toxic to aquatic life.
Precautionary statement(s)

P261 Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P310 Immediately call a POISON CENTER or doctor/ physician.

HMIS Classification

Health hazard: 3
Chronic Health Hazard: *
Flammability: 2
Physical hazards: 0

NFPA Rating

Health hazard: 3
Fire: 2
Reactivity Hazard: 0

Potential Health Effects

Inhalation May be harmful if inhaled. Material is extremely destructive to the tissue of the mucous membranes and upper respiratory tract.

Skin May be harmful if absorbed through skin. Causes skin burns.

Eyes Causes eye burns.

Ingestion Toxic if swallowed.

3. COMPOSITION/INFORMATION ON INGREDIENTS

Synonyms: PITC

Formula: C\textsubscript{7}H\textsubscript{5}NS

Molecular Weight: 135.19 g/mol

<table>
<thead>
<tr>
<th>Component</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Phenyl isothiocyanate</td>
<td></td>
</tr>
<tr>
<td>CAS-No. 103-72-0</td>
<td></td>
</tr>
<tr>
<td>EC-No. 203-138-1</td>
<td>-</td>
</tr>
</tbody>
</table>

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
Take off contaminated clothing and shoes immediately. Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

In case of eye contact
Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician. Continue rinsing eyes during transport to hospital.

If swallowed
Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

5. FIREFIGHTING MEASURES

Suitable extinguishing media
For small (incipient) fires, use media such as "alcohol" foam, dry chemical, or carbon dioxide. For large fires, apply water from as far as possible. Use very large quantities (flooding) of water applied as a mist or spray; solid streams of water may be ineffective. Cool all affected containers with flooding quantities of water.
Special protective equipment for firefighters
Wear self contained breathing apparatus for fire fighting if necessary.

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

Further information
Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES

Personal precautions
Wear respiratory protection. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.

Environmental precautions
Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

Methods and materials for containment and cleaning up
Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13). 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. Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

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. 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. 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.

Immersion protection
Material: Fluorinated rubber
Minimum layer thickness: 0.7 mm
Break through time: > 480 min
Material tested: Vitoject® (Aldrich Z677698, Size M)

Splash protection
Material: butyl-rubber
Minimum layer thickness: 0.3 mm
Break through time: > 30 min
Material tested: Butoject® (Aldrich Z677647, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 873000, e-mail sales@kcl.de, test method: EN374
If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an Industrial Hygienist familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

**Eye protection**
Tightly fitting safety goggles. Faceshield (8-inch minimum). Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

**Skin and 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.

**Hygiene measures**
Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

### 9. PHYSICAL AND CHEMICAL PROPERTIES

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Appearance</strong></td>
<td></td>
</tr>
<tr>
<td>Form</td>
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<tr>
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<tr>
<td><strong>Safety data</strong></td>
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<tr>
<td>pH</td>
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</tr>
<tr>
<td>Melting point/freezing point</td>
<td>Melting point/range: (-21 , ^\circ \text{C} (-6 , ^\circ \text{F})) - lit.</td>
</tr>
<tr>
<td>Boiling point</td>
<td>218 , ^°C (424 , ^°F) - lit.</td>
</tr>
<tr>
<td>Flash point</td>
<td>88 , ^°C (190 , ^°F) - closed cup</td>
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<tr>
<td>Ignition temperature</td>
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<tr>
<td>Autoignition temperature</td>
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<tr>
<td>Lower explosion limit</td>
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<tr>
<td>Upper explosion limit</td>
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<tr>
<td>Vapour pressure</td>
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<tr>
<td>Density</td>
<td>1.132 g/cm^3 at 20 , ^°C (68 , ^°F)</td>
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<tr>
<td>Water solubility</td>
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<tr>
<td>Partition coefficient: n-octanol/water</td>
<td>log Pow: &gt; 3</td>
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<tr>
<td>Relative vapour density</td>
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<tr>
<td>Odour</td>
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<tr>
<td>Odour Threshold</td>
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</tr>
<tr>
<td>Evaporation rate</td>
<td>no data available</td>
</tr>
</tbody>
</table>

### 10. STABILITY AND REACTIVITY

**Chemical stability**
Stable under recommended storage conditions.

**Possibility of hazardous reactions**
no data available

**Conditions to avoid**
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
Other decomposition products - no data available

11. TOXICOLOGICAL INFORMATION

Acute toxicity

Oral LD50
LD50 Oral - mouse - 87 mg/kg
Remarks: Kidney, Ureter, Bladder: Urine volume increased.

Inhalation LC50
no data available

Dermal LD50
no data available

Other information on acute toxicity
no data available

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 vivo - Mammal - Skin
Cytogenetic analysis

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

Teratogenicity

Developmental Toxicity - mouse - Subcutaneous
Effects on Embryo or Fetus: Extra embryonic structures (e.g., placenta, umbilical cord). Effects on Embryo or Fetus: Fetotoxicity (except death, e.g., stunted fetus).

Developmental Toxicity - mouse - Subcutaneous
Specific Developmental Abnormalities: Central nervous system. Specific Developmental Abnormalities: Eye, ear. Specific Developmental Abnormalities: Craniofacial (including nose and tongue).

no data available

Specific target organ toxicity - single exposure (Globally Harmonized System)
no data available
Specific target organ toxicity - repeated exposure (Globally Harmonized System)
no data available

Aspiration hazard
no data available

Potential health effects

Inhalation May be harmful if inhaled. Material is extremely destructive to the tissue of the mucous membranes and upper respiratory tract.

Ingestion Toxic if swallowed.

Skin May be harmful if absorbed through skin. Causes skin burns.

Eyes Causes eye burns.

Signs and Symptoms of Exposure
Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., Cough, Shortness of breath, Headache, Nausea

Synergistic effects
no data available

Additional Information
RTECS: NX9275000

12. ECOLOGICAL INFORMATION

Toxicity
Toxicity to daphnia and other aquatic invertebrates

LC50 - Daphnia magna (Water flea) - 0.1 mg/l - 48 h

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
An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

Toxic to aquatic life.

13. DISPOSAL CONSIDERATIONS

Product
This combustible material may be burned in a chemical incinerator equipped with an afterburner and scrubber. Offer surplus and non-recyclable solutions to a licensed disposal company. 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: 2927 Class: 6.1 (8) Packing group: II
Proper shipping name: Toxic liquids, corrosive, organic, n.o.s. (Phenyl isothiocyanate)
Marine pollutant: No
Poison Inhalation Hazard: No

IMDG
UN number: 2927 Class: 6.1 (8) Packing group: II EMS-No: F-A, S-B
Proper shipping name: TOXIC LIQUID, CORROSIVE, ORGANIC, N.O.S. (Phenyl isothiocyanate)
Marine pollutant: No

IATA
UN number: 2927  Class: 6.1 (8)  Packing group: II
Proper shipping name: Toxic liquid, corrosive, organic, n.o.s. (Phenyl isothiocyanate)

15. REGULATORY INFORMATION

OSHA Hazards
Combustible Liquid, Target Organ Effect, Toxic by ingestion, Corrosive

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
Fire Hazard, Acute Health Hazard, Chronic Health Hazard

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

Pennsylvania Right To Know Components
Phenyl isothiocyanate  CAS-No. 103-72-0

New Jersey Right To Know Components
Phenyl isothiocyanate  CAS-No. 103-72-0

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
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