

# Phenethyl isothiocyanate

sc-205801



The Power is Question

## Material Safety Data Sheet

Hazard Alert Code  
Key:

EXTREME

HIGH

MODERATE

LOW

## Section 1 - CHEMICAL PRODUCT AND COMPANY IDENTIFICATION

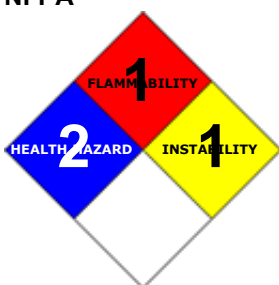
### PRODUCT NAME

Phenethyl isothiocyanate

### STATEMENT OF HAZARDOUS NATURE

CONSIDERED A HAZARDOUS SUBSTANCE ACCORDING TO OSHA 29 CFR 1910.1200.

### NFPA



### SUPPLIER

Company: Santa Cruz Biotechnology, Inc.

Address:

2145 Delaware Ave

Santa Cruz, CA 95060

Telephone: 800.457.3801 or 831.457.3800

Emergency Tel: CHEMWATCH: From within the US and  
Canada: 877-715-9305

Emergency Tel: From outside the US and Canada: +800 2436  
2255 (1-800-CHEMCALL) or call +613 9573 3112

### PRODUCT USE

- Intermediate.

### SYNONYMS

C9-H9-N-S, C9-H9-N-S, C6H5CH2CH2N=C=S, "isothiocyanic acid, phenethyl ester", "benzene, (2-isothiocyanatoethyl)-", "beta-phenethyl isothiocyanate", "phenylethyl isothiocyanate", "beta-phenylethyl isothiocyanate", "2-phenylethyl isothiocyanate", "2-phenylethyl isothiocyanate", "phenylethyl mustard oil"

## Section 2 - HAZARDS IDENTIFICATION

### CANADIAN WHMIS SYMBOLS



### EMERGENCY OVERVIEW

#### RISK

Harmful by inhalation, in contact with skin and if swallowed.

Irritating to eyes, respiratory system and skin.

Very toxic to aquatic organisms.

#### POTENTIAL HEALTH EFFECTS

#### ACUTE HEALTH EFFECTS

#### SWALLOWED

- Accidental ingestion of the material may be harmful; animal experiments indicate that ingestion of less than 150 gram may

be fatal or may produce serious damage to the health of the individual.

#### EYE

- This material can cause eye irritation and damage in some persons.
- Irritation of the eyes may produce a heavy secretion of tears (lachrymation).

#### SKIN

- Skin contact with the material may be harmful; systemic effects may result following absorption.
- This material can cause inflammation of the skin on contact in some persons.
- The material may accentuate any pre-existing dermatitis condition.
- Open cuts, abraded or irritated skin should not be exposed to this material.
- Entry into the blood-stream, through, for example, cuts, abrasions or lesions, may produce systemic injury with harmful effects. Examine the skin prior to the use of the material and ensure that any external damage is suitably protected.

#### INHALED

- Inhalation of aerosols (mists, fumes), generated by the material during the course of normal handling, may be harmful.
- The material can cause respiratory irritation in some persons. The body's response to such irritation can cause further lung damage.
- Inhalation hazard is increased at higher temperatures.

#### CHRONIC HEALTH EFFECTS

- Long-term exposure to respiratory irritants may result in disease of the airways involving difficult breathing and related systemic problems.

Limited evidence suggests that repeated or long-term occupational exposure may produce cumulative health effects involving organs or biochemical systems.

There is some evidence that inhaling this product is more likely to cause a sensitization reaction in some persons compared to the general population.

There is limited evidence that, skin contact with this product is more likely to cause a sensitization reaction in some persons compared to the general population.

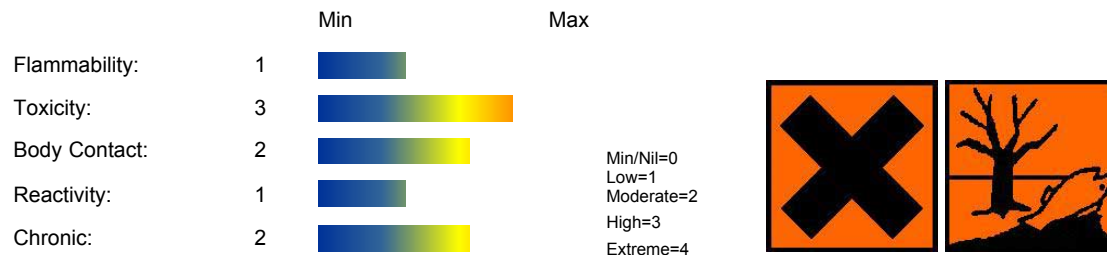
Isothiocyanates have been used as inducers of apoptosis (programmed cell death).

Isothiocyanate-induced apoptosis may suppress the growth of pre-clinical tumours and contribute to the well-established decreased cancer incidence associated with a vegetable-rich diet. Under physiological conditions, isothiocyanates react rapidly with cysteinyl thiol groups to form S-thiocarbamoylcysteine derivatives - which is reversible, and slowly with amino groups to form thioureas. A competing reaction is the hydrolysis of isothiocyanates to corresponding monothiocarbamates and fragmentation to the related amines.

The chemopreventive activity of dietary isothiocyanates has been attributed to the decreased activation and increased conjugation of excretion of carcinogens. Isothiocyanates and their cysteine conjugates inhibited cytochrome P450 isozymes 1A1, 1A2, 2B1 and 2E1. They also induced increased activities of enzymes involved in the detoxification and conjugation of carcinogens for elimination: glutathione S-transferases, quinone reductase, epoxide hydrolase and UDP glucuronosyl transferases. A further feature of the pharmacological activity of dietary isothiocyanates and related S-(N-thiocarbamoyl)cysteine derivatives was their anticancer activity. Inhibition of tumour growth in pre-clinical development by isothiocyanates may contribute to the association of decreased cancer incidence with dietary glucosinolate consumption. Cruciferous vegetables are the major dietary source of naturally occurring thioglucosides or glucosinolates. Glucosinolates are degraded non-enzymatically and enzymatically during food preparation, cooking and chewing. repeated exposure may cause sensitization and/or allergic reactions.

## Section 3 - COMPOSITION / INFORMATION ON INGREDIENTS

### HAZARD RATINGS



| NAME                     | CAS RN    | %   |
|--------------------------|-----------|-----|
| phenethyl isothiocyanate | 2257-09-2 | >98 |

## Section 4 - FIRST AID MEASURES

### SWALLOWED

- IF SWALLOWED, REFER FOR MEDICAL ATTENTION, WHERE POSSIBLE, WITHOUT DELAY.
- Where Medical attention is not immediately available or where the patient is more than 15 minutes from a hospital or unless instructed otherwise:
  - For advice, contact a Poisons Information Center or a doctor.
  - Urgent hospital treatment is likely to be needed.
  - If conscious, give water to drink.
  - INDUCE vomiting with fingers down the back of the throat, ONLY IF CONSCIOUS. Lean patient forward or place on left side (head-down position, if possible) to maintain open airway and prevent aspiration.

NOTE: Wear a protective glove when inducing vomiting by mechanical means.

- In the mean time, qualified first-aid personnel should treat the patient following observation and employing supportive measures as indicated by the patient's condition.
- If the services of a medical officer or medical doctor are readily available, the patient should be placed in his/her care and a copy of the MSDS should be provided. Further action will be the responsibility of the medical specialist.
- If medical attention is not available on the worksite or surroundings send the patient to a hospital together with a copy of

the MSDS.

## EYE

- If this product comes in contact with the eyes:
  - Wash out immediately with fresh running water.
  - Ensure complete irrigation of the eye by keeping eyelids apart and away from eye and moving the eyelids by occasionally lifting the upper and lower lids.
  - If pain persists or recurs seek medical attention.
  - Removal of contact lenses after an eye injury should only be undertaken by skilled personnel.

## SKIN

- If skin contact occurs:
  - Immediately remove all contaminated clothing, including footwear
  - Flush skin and hair with running water (and soap if available).
  - Seek medical attention in event of irritation.

## INHALED

- - If fumes or combustion products are inhaled remove from contaminated area.
  - Lay patient down. Keep warm and rested.
  - Prostheses such as false teeth, which may block airway, should be removed, where possible, prior to initiating first aid procedures.
  - Apply artificial respiration if not breathing, preferably with a demand valve resuscitator, bag-valve mask device, or pocket mask as trained. Perform CPR if necessary.
  - Transport to hospital, or doctor, without delay.

## NOTES TO PHYSICIAN

- for poisons (where specific treatment regime is absent):

### BASIC TREATMENT

- Establish a patent airway with suction where necessary.
- Watch for signs of respiratory insufficiency and assist ventilation as necessary.
- Administer oxygen by non-rebreather mask at 10 to 15 l/min.
- Monitor and treat, where necessary, for pulmonary edema .
- Monitor and treat, where necessary, for shock.
- Anticipate seizures .
- DO NOT use emetics. Where ingestion is suspected rinse mouth and give up to 200 ml water (5 ml/kg recommended) for dilution where patient is able to swallow, has a strong gag reflex and does not drool.

### ADVANCED TREATMENT

- Consider orotracheal or nasotracheal intubation for airway control in unconscious patient or where respiratory arrest has occurred.
- Positive-pressure ventilation using a bag-valve mask might be of use.
- Monitor and treat, where necessary, for arrhythmias.
- Start an IV D5W TKO. If signs of hypovolemia are present use lactated Ringers solution. Fluid overload might create complications.
- Drug therapy should be considered for pulmonary edema.
- Hypotension with signs of hypovolemia requires the cautious administration of fluids. Fluid overload might create complications.
- Treat seizures with diazepam.
- Proparacaine hydrochloride should be used to assist eye irrigation.

BRONSTEIN, A.C. and CURRANCE, P.L.

EMERGENCY CARE FOR HAZARDOUS MATERIALS EXPOSURE: 2nd Ed. 1994.

Treat symptomatically.

## Section 5 - FIRE FIGHTING MEASURES

|                             |               |
|-----------------------------|---------------|
| Vapour Pressure (mmHG):     | Not available |
| Upper Explosive Limit (%):  | Not available |
| Specific Gravity (water=1): | 1.094         |
| Lower Explosive Limit (%):  | Not available |

## EXTINGUISHING MEDIA

- - DO NOT use water.

## FIRE FIGHTING

- - Alert Emergency Responders and tell them location and nature of hazard.
  - Wear full body protective clothing with breathing apparatus.
  - Prevent, by any means available, spillage from entering drains or water course.
  - Use fire fighting procedures suitable for surrounding area.
  - DO NOT approach containers suspected to be hot.
  - Cool fire exposed containers with water spray from a protected location.
  - If safe to do so, remove containers from path of fire.
  - Equipment should be thoroughly decontaminated after use.

## GENERAL FIRE HAZARDS/HAZARDOUS COMBUSTIBLE PRODUCTS

- - Combustible.

- Slight fire hazard when exposed to heat or flame.
- Heating may cause expansion or decomposition leading to violent rupture of containers.
- On combustion, may emit toxic fumes of carbon monoxide (CO).
- May emit acrid smoke.
- Mists containing combustible materials may be explosive.

Combustion products include: carbon dioxide (CO<sub>2</sub>), nitrogen oxides (NO<sub>x</sub>), sulfur oxides (SO<sub>x</sub>), other pyrolysis products typical of burning organic material.  
May emit poisonous fumes.

#### FIRE INCOMPATIBILITY

- Avoid contamination with oxidizing agents i.e. nitrates, oxidizing acids, chlorine bleaches, pool chlorine etc. as ignition may result.

#### PERSONAL PROTECTION

Glasses:

Chemical goggles.

Gloves:

Respirator:

Type A Filter of sufficient capacity

## Section 6 - ACCIDENTAL RELEASE MEASURES

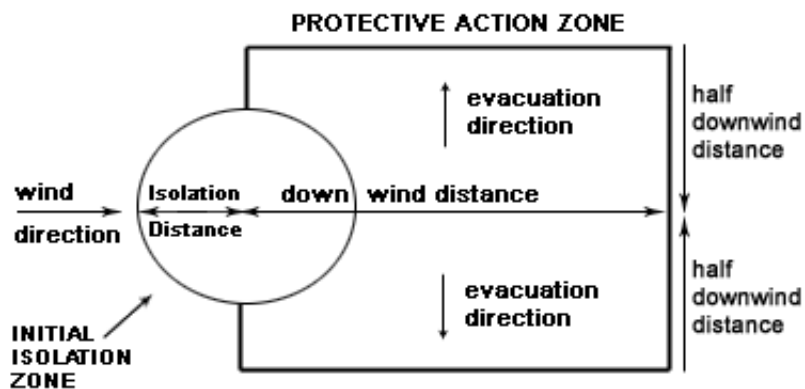
#### MINOR SPILLS

- 
- Remove all ignition sources.
- Clean up all spills immediately.
- Avoid breathing vapors and contact with skin and eyes.
- Control personal contact by using protective equipment.
- Contain and absorb spill with sand, earth, inert material or vermiculite.
- Wipe up.
- Place in a suitable labeled container for waste disposal.

#### MAJOR SPILLS

- 
- Clear area of personnel and move upwind.
- Alert Emergency Responders and tell them location and nature of hazard.
- Wear full body protective clothing with breathing apparatus.
- Prevent, by any means available, spillage from entering drains or water course.
- Stop leak if safe to do so.
- Contain spill with sand, earth or vermiculite.
- Collect recoverable product into labeled containers for recycling.
- Neutralize/decontaminate residue.
- Collect solid residues and seal in labeled drums for disposal.
- Wash area and prevent runoff into drains.
- After clean up operations, decontaminate and launder all protective clothing and equipment before storing and re-using.
- If contamination of drains or waterways occurs, advise emergency services.

#### PROTECTIVE ACTIONS FOR SPILL



From US Emergency Response Guide 2000 Guide 153

#### SMALL SPILLS

| Name   | Isolation Distance | Downwind Day      | Protection Night  |
|--|--------------------|-------------------|-------------------|
| Toxic liquid, organic, n.o.s. (Inhalation Hazard Zone A)                                 | 700 ft (215 m)     | 1.2 mile (1.9 km) | 2.7 mile (4.3 km) |
| Toxic liquid, organic, n.o.s. (Inhalation Hazard Zone B)                                 | 200 ft (60 m)      | 0.2 mile (0.3 km) | 0.7 mile (1.1 km) |
| Toxic liquid, organic, n.o.s. (when Inhalation Hazard is on a package or shipping paper) | 700 ft (215 m)     | 1.2 mile (1.9 km) | 2.7 mile (4.3 km) |

From IERG (Canada/Australia)

|                              |            |
|------------------------------|------------|
| Isolation Distance           | 25 meters  |
| Downwind Protection Distance | 250 meters |

## LARGE SPILLS

| Name   | Isolation Distance | Downwind Day          | Protection Night      |
|--|--------------------|-----------------------|-----------------------|
| Toxic liquid, organic, n.o.s. (Inhalation Hazard Zone A)                                 | 3000 ft (915 m)    | (7.0+ mile (11.0+ km) | (7.0+ mile (11.0+ km) |
| Toxic liquid, organic, n.o.s. (Inhalation Hazard Zone B)                                 | 600 ft (185 m)     | 1 mile (1.6 km)       | 2.5 mile (4 km)       |
| Toxic liquid, organic, n.o.s. (when Inhalation Hazard is on a package or shipping paper) | 3000 ft (915 m)    | (7.0+ mile (11.0+ km) | (7.0+ mile (11.0+ km) |

## FOOTNOTES

1 PROTECTIVE ACTION ZONE is defined as the area in which people are at risk of harmful exposure. This zone assumes that random changes in wind direction confines the vapour plume to an area within 30 degrees on either side of the predominant wind direction, resulting in a crosswind protective action distance equal to the downwind protective action distance.

2 PROTECTIVE ACTIONS should be initiated to the extent possible, beginning with those closest to the spill and working away from the site in the downwind direction. Within the protective action zone a level of vapour concentration may exist resulting in nearly all unprotected persons becoming incapacitated and unable to take protective action and/or incurring serious or irreversible health effects.

3 INITIAL ISOLATION ZONE is determined as an area, including upwind of the incident, within which a high probability of localised wind reversal may expose nearly all persons without appropriate protection to life-threatening concentrations of the material.

4 SMALL SPILLS involve a leaking package of 200 litres (55 US gallons) or less, such as a drum (jerrican or box with inner containers). Larger packages leaking less than 200 litres and compressed gas leaking from a small cylinder are also considered "small spills". LARGE SPILLS involve many small leaking packages or a leaking package of greater than 200 litres, such as a cargo tank, portable tank or a "one-tonne" compressed gas cylinder.

5 Guide 153 is taken from the US DOT emergency response guide book.

6 IERG information is derived from CANUTEC - Transport Canada.

## ACUTE EXPOSURE GUIDELINE LEVELS (AEGL) (in ppm)

AEGL 1: The airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, could experience notable discomfort, irritation, or certain asymptomatic nonsensory effects. However, the effects are not disabling and are transient and reversible upon cessation of exposure.

AEGL 2: The airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, could experience irreversible or other serious, long-lasting adverse health effects or an impaired ability to escape.

AEGL 3: The airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, could experience life-threatening health effects or death.

## Section 7 - HANDLING AND STORAGE

### PROCEDURE FOR HANDLING

- Avoid all personal contact, including inhalation.
- Wear protective clothing when risk of exposure occurs.
- Use in a well-ventilated area.
- Prevent concentration in hollows and sumps.
- DO NOT enter confined spaces until atmosphere has been checked.
- DO NOT allow material to contact humans, exposed food or food utensils.
- Avoid contact with incompatible materials.
- When handling, DO NOT eat, drink or smoke.
- Keep containers securely sealed when not in use.
- Avoid physical damage to containers.
- Always wash hands with soap and water after handling.
- Work clothes should be laundered separately.
- Launder contaminated clothing before re-use.
- Use good occupational work practice.
- Observe manufacturer's storing and handling recommendations.
- Atmosphere should be regularly checked against established exposure standards to ensure safe working conditions are maintained.
- DO NOT allow clothing wet with material to stay in contact with skin

### RECOMMENDED STORAGE METHODS

- Lined metal can, Lined metal pail/drum
- Plastic pail
- Polyliner drum
- Packing as recommended by manufacturer.
- Check all containers are clearly labeled and free from leaks.

For low viscosity materials

- Drums and jerricans must be of the non-removable head type.
- Where a can is to be used as an inner package, the can must have a screwed enclosure.

For materials with a viscosity of at least 2680 cSt. (23 deg. C) and solids (between 15 C deg. and 40 deg C.):

- Removable head packaging;
- Cans with friction closures and
- low pressure tubes and cartridges may be used.

- Where combination packages are used, and the inner packages are of glass, there must be sufficient inert cushioning material in contact with inner and outer packages \* . - In addition, where inner packagings are glass and contain liquids of packing group I and II there must be sufficient inert absorbent to absorb any spillage \*. - \* unless the outer packaging is a

close fitting molded plastic box and the substances are not incompatible with the plastic. All inner and sole packagings for substances that have been assigned to Packaging Groups I or II on the basis of inhalation toxicity criteria, must be hermetically sealed.

### STORAGE REQUIREMENTS

- Store in original containers.
- Keep containers securely sealed.
- Store in a cool, dry, well-ventilated area.
- Store away from incompatible materials and foodstuff containers.
- Protect containers against physical damage and check regularly for leaks.
- Observe manufacturer's storing and handling recommendations.

### SAFE STORAGE WITH OTHER CLASSIFIED CHEMICALS



X: Must not be stored together

O: May be stored together with specific preventions

+: May be stored together

## Section 8 - EXPOSURE CONTROLS / PERSONAL PROTECTION

### EXPOSURE CONTROLS

The following materials had no OELs on our records

- phenethyl isothiocyanate: CAS:2257-09-2

### MATERIAL DATA

PHENETHYL ISOTHIOCYANATE:

■ Sensory irritants are chemicals that produce temporary and undesirable side-effects on the eyes, nose or throat. Historically occupational exposure standards for these irritants have been based on observation of workers' responses to various airborne concentrations. Present day expectations require that nearly every individual should be protected against even minor sensory irritation and exposure standards are established using uncertainty factors or safety factors of 5 to 10 or more. On occasion animal no-observable-effect-levels (NOEL) are used to determine these limits where human results are unavailable. An additional approach, typically used by the TLV committee (USA) in determining respiratory standards for this group of chemicals, has been to assign ceiling values (TLV C) to rapidly acting irritants and to assign short-term exposure limits (TLV STELs) when the weight of evidence from irritation, bioaccumulation and other endpoints combine to warrant such a limit. In contrast the MAK Commission (Germany) uses a five-category system based on intensive odour, local irritation, and elimination half-life. However this system is being replaced to be consistent with the European Union (EU) Scientific Committee for Occupational Exposure Limits (SCOEL); this is more closely allied to that of the USA.

OSHA (USA) concluded that exposure to sensory irritants can:

- cause inflammation
- cause increased susceptibility to other irritants and infectious agents
- lead to permanent injury or dysfunction
- permit greater absorption of hazardous substances and
- acclimate the worker to the irritant warning properties of these substances thus increasing the risk of overexposure.

### PERSONAL PROTECTION



Consult your EHS staff for recommendations

#### EYE

- Safety glasses with side shields.
- Chemical goggles.
- Contact lenses pose a special hazard; soft lenses may absorb irritants and all lenses concentrate them. DO NOT wear contact lenses.

#### HANDS/FEET

■ Wear chemical protective gloves, eg. PVC.

Wear safety footwear or safety gumboots, eg. Rubber.

NOTE: The material may produce skin sensitization in predisposed individuals. Care must be taken, when removing gloves and other protective equipment, to avoid all possible skin contact.

Suitability and durability of glove type is dependent on usage. Important factors in the selection of gloves include: such as:

- frequency and duration of contact,
- chemical resistance of glove material,
- glove thickness and



- dexterity

Select gloves tested to a relevant standard (e.g. Europe EN 374, US F739).

- When prolonged or frequently repeated contact may occur, a glove with a protection class of 5 or higher (breakthrough time greater than 240 minutes according to EN 374) is recommended.
- When only brief contact is expected, a glove with a protection class of 3 or higher (breakthrough time greater than 60 minutes according to EN 374) is recommended.
- Contaminated gloves should be replaced.

Gloves must only be worn on clean hands. After using gloves, hands should be washed and dried thoroughly. Application of a non-perfumed moisturiser is recommended.

- Neoprene gloves

## OTHER

- 
- Overalls.
- Eyewash unit.
- Barrier cream.
- Skin cleansing cream.

## RESPIRATOR

■ Selection of the Class and Type of respirator will depend upon the level of breathing zone contaminant and the chemical nature of the contaminant. Protection Factors (defined as the ratio of contaminant outside and inside the mask) may also be important.

| Breathing Zone Level ppm (volume) | Maximum Protection Factor | Half-face Respirator | Full-Face Respirator |
|-----------------------------------|---------------------------|----------------------|----------------------|
| 1000                              | 10                        | A-1                  | -                    |
| 1000                              | 50                        | -                    | A-1                  |
| 5000                              | 50                        | Airline*             | -                    |
| 5000                              | 100                       | -                    | A-2                  |
| 10000                             | 100                       | -                    | A-3                  |
|                                   | 100+                      |                      | Airline* *           |

\* - Continuous Flow \*\* - Continuous-flow or positive pressure demand.

The local concentration of material, quantity and conditions of use determine the type of personal protective equipment required.

Use appropriate NIOSH-certified respirator based on informed professional judgement. In conditions where no reasonable estimate of exposure can be made, assume the exposure is in a concentration IDLH and use NIOSH-certified full face pressure demand SCBA with a minimum service life of 30 minutes, or a combination full facepiece pressure demand SAR with auxiliary self-contained air supply. Respirators provided only for escape from IDLH atmospheres shall be NIOSH-certified for escape from the atmosphere in which they will be used.

## ENGINEERING CONTROLS

■ Local exhaust ventilation usually required. If risk of overexposure exists, wear an approved respirator. Correct fit is essential to obtain adequate protection an approved self contained breathing apparatus (SCBA) may be required in some situations. Provide adequate ventilation in warehouse or closed storage area.

Air contaminants generated in the workplace possess varying "escape" velocities which, in turn, determine the "capture velocities" of fresh circulating air required to effectively remove the contaminant.

| Type of Contaminant:  | Air Speed:                   |
|---|------------------------------|
| solvent, vapors, degreasing etc., evaporating from tank (in still air).   | 0.25-0.5 m/s (50-100 f/min.) |
| aerosols, fumes from pouring operations, intermittent container filling, low speed conveyer transfers, welding, spray drift, plating acid fumes, pickling (released at low velocity into zone of active generation) | 0.5-1 m/s (100-200 f/min.)   |
| direct spray, spray painting in shallow booths, drum filling, conveyer loading, crusher dusts, gas discharge (active generation into zone of rapid air motion)  | 1-2.5 m/s (200-500 f/min.)   |
| grinding, abrasive blasting, tumbling, high speed wheel generated dusts (released at high initial velocity into zone of very high rapid air motion).  | 2.5-10 m/s (500-2000 f/min.) |

Within each range the appropriate value depends on:

| Lower end of the range                                     | Upper end of the range           |
|--|----------------------------------|
| 1: Room air currents minimal or favorable to capture       | 1: Disturbing room air currents  |
| 2: Contaminants of low toxicity or of nuisance value only. | 2: Contaminants of high toxicity |
| 3: Intermittent, low production.                           | 3: High production, heavy use    |
| 4: Large hood or large air mass in motion                  | 4: Small hood-local control only |

Simple theory shows that air velocity falls rapidly with distance away from the opening of a simple extraction pipe. Velocity generally decreases with the square of distance from the extraction point (in simple cases). Therefore the air speed at the extraction point should be adjusted, accordingly, after reference to distance from the contaminating source. The air velocity at the extraction fan, for example, should be a minimum of 1-2 m/s (200-400 f/min) for extraction of solvents generated in a tank 2 meters distant from the extraction point. Other mechanical considerations, producing performance deficits within the extraction apparatus, make it essential that theoretical air velocities are multiplied by factors of 10 or more when extraction systems are installed or used.

## Section 9 - PHYSICAL AND CHEMICAL PROPERTIES

### PHYSICAL PROPERTIES

Liquid.

|       |        |                  |        |
|-------|--------|------------------|--------|
| State | Liquid | Molecular Weight | 163.24 |
|-------|--------|------------------|--------|

|                           |                    |                                |                 |
|---------------------------|--------------------|--------------------------------|-----------------|
| Melting Range (°F)        | Not available      | Viscosity                      | Not Available   |
| Boiling Range (°F)        | 282.2- 284 (11 mm) | Solubility in water (g/L)      | Reacts          |
| Flash Point (°F)          | >230               | pH (1% solution)               | Not applicable. |
| Decomposition Temp (°F)   | Not available.     | pH (as supplied)               | Not applicable  |
| Autoignition Temp (°F)    | Not available      | Vapour Pressure (mmHG)         | Not available   |
| Upper Explosive Limit (%) | Not available      | Specific Gravity (water=1)     | 1.094           |
| Lower Explosive Limit (%) | Not available      | Relative Vapor Density (air=1) | >1              |
| Volatile Component (%vol) | Not available      | Evaporation Rate               | Not available   |

## APPEARANCE

Yellow liquid, does not mix with water.

## Section 10 - CHEMICAL STABILITY

### CONDITIONS CONTRIBUTING TO INSTABILITY

- 
- Presence of incompatible materials.
- Product is considered stable.
- Hazardous polymerization will not occur.

### STORAGE INCOMPATIBILITY

- 
- Contact with acids produces toxic fumes

Isothiocyanates ( thioisocyanates):

- are incompatible with many classes of compounds, reacting exothermically to release toxic gases. Reactions with amines, strong bases, aldehydes, alcohols, alkali metals, ketones, mercaptans, strong oxidisers, hydrides, phenols, and peroxides can cause vigorous releases of heat.
- Acids and bases initiate polymerisation reactions in these materials

Avoid reaction with oxidizing agents.

- NOTE: May develop pressure in containers; open carefully. Vent periodically.
- Segregate from alcohol, water.

For incompatible materials - refer to Section 7 - Handling and Storage.

## Section 11 - TOXICOLOGICAL INFORMATION

phenethyl isothiocyanate

### TOXICITY AND IRRITATION

- unless otherwise specified data extracted from RTECS - Register of Toxic Effects of Chemical Substances.

| TOXICITY                             | IRRITATION   |
|--------------------------------------|--------------|
| Oral (mouse) LD50: 700 mg/kg         | Nil Reported |
| Subcutaneous (mouse) LD50: 150 mg/kg |              |

Intravenous (mouse) LD50: 50 mg/kg

■ Asthma-like symptoms may continue for months or even years after exposure to the material ceases. This may be due to a non-allergenic condition known as reactive airways dysfunction syndrome (RADS) which can occur following exposure to high levels of highly irritating compound. Key criteria for the diagnosis of RADS include the absence of preceding respiratory disease, in a non-atopic individual, with abrupt onset of persistent asthma-like symptoms within minutes to hours of a documented exposure to the irritant. A reversible airflow pattern, on spirometry, with the presence of moderate to severe bronchial hyperreactivity on methacholine challenge testing and the lack of minimal lymphocytic inflammation, without eosinophilia, have also been included in the criteria for diagnosis of RADS. RADS (or asthma) following an irritating inhalation is an infrequent disorder with rates related to the concentration of and duration of exposure to the irritating substance. Industrial bronchitis, on the other hand, is a disorder that occurs as result of exposure due to high concentrations of irritating substance (often particulate in nature) and is completely reversible after exposure ceases. The disorder is characterised by dyspnea, cough and mucus production.

## Section 12 - ECOLOGICAL INFORMATION

Refer to data for ingredients, which follows:

PHENETHYL ISOTHIOCYANATE:

- Very toxic to aquatic organisms.
  - Do NOT allow product to come in contact with surface waters or to intertidal areas below the mean high water mark. Do not contaminate water when cleaning equipment or disposing of equipment wash-waters.
- Wastes resulting from use of the product must be disposed of on site or at approved waste sites.
- For aliphatic isothiocyanates (ITCs).

The DT50 of ITCs in soil are very short. Germination tests with weed seeds in aqueous ITC solutions showed, that aryl-ITCs were the most suppressive compounds. Within the alkyl-ITCs, the activity decreased with increasing molecular mass. The susceptibility of different weed species to ITCs mainly depended on seed size. Smaller seeds tended to be more sensitive. Further studies demonstrated a high biological activity of ITCs in the vapor phase. n-Butyl-ITC was more suppressive in the vapor phase than in aqueous solution, while 2-phenylethyl-ITC showed the opposite effect.

Jan Peterson et al: Agronomy Journal 93: 2001, pp 37-43

ITCs can act as Michael-type acceptors with N-hydro-C-mercapto-addition to cellular thiols as a molecular mechanism of action. Comparison of both aquatic toxicity and reactivity among the analogues revealed that derivatives with a branch



hydrocarbon moiety, especially branched in the  $\beta$ -position were less toxic and less reactive. In contrast, the di-isothiocyanate and the allyl and propargyl derivatives are more toxic than their 1-alkyl homologues. The toxicity and reactivity differences are consistent but except for the tert-butyl-derivative not remarkable. The differences are due to variations in steric hindrance at the reaction center.

T Wayne Schultz et al; Environmental Toxicology and Pharmacology Vol 23, Jan 2007 pp 10-17.

■ DO NOT discharge into sewer or waterways.

### Ecotoxicity

|                          |                         |                  |                 |          |
|--------------------------|-------------------------|------------------|-----------------|----------|
| Ingredient               | Persistence: Water/Soil | Persistence: Air | Bioaccumulation | Mobility |
| phenethyl isothiocyanate | HIGH                    |                  | LOW             | MED      |

## Section 13 - DISPOSAL CONSIDERATIONS

### Disposal Instructions

All waste must be handled in accordance with local, state and federal regulations.

! Puncture containers to prevent re-use and bury at an authorized landfill.

Legislation addressing waste disposal requirements may differ by country, state and/ or territory. Each user must refer to laws operating in their area. In some areas, certain wastes must be tracked.

A Hierarchy of Controls seems to be common - the user should investigate:

- Reduction,
- Reuse
- Recycling
- Disposal (if all else fails)

This material may be recycled if unused, or if it has not been contaminated so as to make it unsuitable for its intended use. If it has been contaminated, it may be possible to reclaim the product by filtration, distillation or some other means. Shelf life considerations should also be applied in making decisions of this type. Note that properties of a material may change in use, and recycling or reuse may not always be appropriate.

DO NOT allow wash water from cleaning equipment to enter drains. Collect all wash water for treatment before disposal.

- Recycle wherever possible or consult manufacturer for recycling options.
- Consult Waste Management Authority for disposal.
- Bury or incinerate residue at an approved site.
- Recycle containers if possible, or dispose of in an authorized landfill.

## Section 14 - TRANSPORTATION INFORMATION



DOT:

|  |        |  |                           |
|--|--------|--|---------------------------|
| Symbols:                                   | None   | Hazard class or Division:                      | 6.1                       |
| Identification Numbers:                    | UN2810 | PG:  | II                        |
| Label Codes:                               | 6.1    | Special provisions:                            | IB2, T11, TP2, TP13, TP27 |
| Packaging: Exceptions:                     | 153    | Packaging: Non-bulk:                           | 202                       |
| Packaging: Exceptions:                     | 153    | Quantity limitations: Passenger aircraft/rail: | 5 L                       |
| Quantity Limitations: Cargo aircraft only: | 60 L   | Vessel stowage: Location:                      | B                         |
| Vessel stowage: Other:                     | 40     |  |                           |

Hazardous materials descriptions and proper shipping names:

Toxic, liquids, organic, n.o.s.

### Air Transport IATA:

|                     |      |                    |      |
|---------------------|------|--------------------|------|
| ICAO/IATA Class:    | 6.1  | ICAO/IATA Subrisk: | None |
| UN/ID Number:       | 2810 | Packing Group:     | II   |
| Special provisions: | A3   |                    |      |

Shipping Name: TOXIC LIQUID, ORGANIC, N.O.S. \*(CONTAINS PHENETHYL ISOTHIOCYANATE)

### Maritime Transport IMDG:

|                     |         |                     |      |
|---------------------|---------|---------------------|------|
| IMDG Class:         | 6.1     | IMDG Subrisk:       | None |
| UN Number:          | 2810    | Packing Group:      | II   |
| EMS Number:         | F-A,S-A | Special provisions: | 274  |
| Limited Quantities: | 100 ml  |                     |      |

Shipping Name: TOXIC LIQUID, ORGANIC, N.O.S.(contains phenethyl isothiocyanate)

## Section 15 - REGULATORY INFORMATION

phenethyl isothiocyanate (CAS: 2257-09-2) is found on the following regulatory lists;

## Section 16 - OTHER INFORMATION

### LIMITED EVIDENCE

- Cumulative effects may result following exposure\*.
- Possible respiratory and skin sensitizer\*.

\* (limited evidence).

*Reasonable care has been taken in the preparation of this information, but the author makes no warranty of merchantability or any other warranty, expressed or implied, with respect to this information. The author makes no representations and assumes no liability for any direct, incidental or consequential damages resulting from its use. For additional technical information please call our toxicology department on +800 CHEMCALL.*

- Classification of the mixture and its individual components has drawn on official and authoritative sources as well as independent review by the Chemwatch Classification committee using available literature references.

A list of reference resources used to assist the committee may be found at:  
[www.chemwatch.net/references](http://www.chemwatch.net/references).

- The (M)SDS is a Hazard Communication tool and should be used to assist in the Risk Assessment. Many factors determine whether the reported Hazards are Risks in the workplace or other settings. Risks may be determined by reference to Exposures Scenarios. Scale of use, frequency of use and current or available engineering controls must be considered.

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