1-Dodecanethiol

sc-255824

Section 1 - CHEMICAL PRODUCT AND COMPANY IDENTIFICATION

PRODUCT NAME
1-Dodecanethiol

STATEMENT OF HAZARDOUS NATURE

NFPA

SUPPLIER
Santa Cruz Biotechnology, Inc.
2145 Delaware Avenue
Santa Cruz, California 95060
800.457.3801 or 831.457.3800

EMERGENCY:
ChemWatch
Within the US & Canada: 877-715-9305
Outside the US & Canada: +800 2436 2255
(1-800-CHEMCALL) or call +613 9673 3112

SYNONYMS

Section 2 - HAZARDS IDENTIFICATION

CHEMWATCH HAZARD RATINGS

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Min</th>
<th>Max</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flammability</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>Toxicity</td>
<td>2</td>
<td></td>
</tr>
<tr>
<td>Body Contact</td>
<td>3</td>
<td></td>
</tr>
<tr>
<td>Reactivity</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>Chronic</td>
<td>2</td>
<td></td>
</tr>
</tbody>
</table>

Canadian WHMIS Symbols

1 of 8
EMERGENCY OVERVIEW

RISK
Risk of serious damage to eyes. May cause SENSITISATION by inhalation and skin contact. Irritating to respiratory system and skin.

POTENTIAL HEALTH EFFECTS

ACUTE HEALTH EFFECTS

SWALLOWED
- Although ingestion is not thought to produce harmful effects, the material may still be damaging to the health of the individual following ingestion, especially where pre-existing organ (e.g. liver, kidney) damage is evident.

EYE
- If applied to the eyes, this material causes severe eye damage.

SKIN
- This material can cause inflammation of the skin on contact in some persons.
- The material may accentuate any pre-existing dermatitis condition.
- Skin contact is not thought to have harmful health effects, however the material may still produce health damage following entry through wounds, lesions or abrasions.
- 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
- The material can cause respiratory irritation in some persons. The body's response to such irritation can cause further lung damage.
- Inhalation of aerosols (mists, fumes), generated by the material during the course of normal handling, may be damaging to the health of the individual.
- Thiols (particularly ethyl mercaptan) produce lethargy or sleepiness. Exposure to high levels may result in nausea, vomiting, restlessness, muscle incoordination and or paralysis, bluing of skin, depression of breathing, coma and death.

CHRONIC HEALTH EFFECTS
- Long-term exposure to respiratory irritants may result in disease of the airways involving difficult breathing and related systemic problems. Inhaling this product is more likely to cause a sensitization reaction in some persons compared to the general population.
- Skin contact with the material is more likely to cause a sensitization reaction in some persons compared to the general population.
- Limited evidence suggests that repeated or long-term occupational exposure may produce cumulative health effects involving organs or biochemical systems.
- Chronic exposure to mercaptans may result in damage to the lungs, kidneys and liver.
- Skin irritation and sensitisation are common for example in the shoe industry following occupational use. It is postulated that synergistic effects may result following exposure to other chemicals commonly used with synthetic rubber compounds. Workers exposed to mixtures with polychloroprene latexes show a significant increase in the number of chromosome aberrations in the peripheral blood. Rabbits exposed to mixtures encountered in synthetic rubber compounds show increases in the occurrence of chromosomal aberrations of the brain.

Section 3 - COMPOSITION / INFORMATION ON INGREDIENTS

<table>
<thead>
<tr>
<th>NAME</th>
<th>CAS RN</th>
<th>%</th>
</tr>
</thead>
<tbody>
<tr>
<td>n-dodecyl mercaptan</td>
<td>112-55-0</td>
<td>98</td>
</tr>
</tbody>
</table>

Section 4 - FIRST AID MEASURES

SWALLOWED
- Immediately give a glass of water. First aid is not generally required. If in doubt, contact a Poisons Information Center or a doctor.

EYE
- If this product comes in contact with the eyes: Immediately hold eyelids apart and flush the eye continuously with 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.

SKIN
- If skin contact occurs: Immediately remove all contaminated clothing, including footwear. Flush skin and hair with running water (and soap if available).

INHALED
- If fumes or combustion products are inhaled remove from contaminated area. Lay patient down. Keep warm and rested.
NOTES TO PHYSICIAN

- For exposures involving sulfides and hydrogen sulfide (including gastric acid decomposition products of alkaline sulfides).
  - Hydrogen sulfide anion produces its major toxic effect through inhibition of cytochrome oxidases.
  - Symptoms include profuse salivation, nausea, vomiting and diarrhea. Central nervous effects may include giddiness, headache, vertigo, amnesia, confusion and unconsciousness. Tachypnea, palpitation, tachycardia, arrhythmia, sweating, weakness and muscle cramps may also indicate over-exposures.

Section 5 - FIRE FIGHTING MEASURES

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vapour Pressure (mmHG)</td>
<td>Not available</td>
</tr>
<tr>
<td>Upper Explosive Limit (%)</td>
<td>Not available</td>
</tr>
<tr>
<td>Specific Gravity (water=1)</td>
<td>0.845</td>
</tr>
<tr>
<td>Lower Explosive Limit (%)</td>
<td>Not available</td>
</tr>
</tbody>
</table>

**EXTINGUISHING MEDIA**

- Dry chemical powder.
- BCF (where regulations permit).

**FIRE FIGHTING**

- Alert Emergency Responders and tell them location and nature of hazard.
- Wear full body protective clothing with breathing apparatus.
- When any large container (including road and rail tankers) is involved in a fire, consider evacuation by 100 metres in all directions.

**GENERAL FIRE HAZARDS/HAZARDOUS COMBUSTIBLE PRODUCTS**

- Combustible.
- Slight fire hazard when exposed to heat or flame.

Combustion products include: carbon dioxide (CO₂), sulfur oxides (SOₓ), hydrogen sulfide (H₂S), other pyrolysis products typical of burning organic material.

**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 AB-P Filter of sufficient capacity

Section 6 - ACCIDENTAL RELEASE MEASURES

**MINOR SPILLS**

- **WARNING:** Never use dry, powdered hypochlorite or other strong oxidizer for mercaptan spills, as autoignition can occur.
  - Clean up all spills immediately.
  - Avoid breathing vapors and contact with skin and eyes.

**MAJOR SPILLS**

- Moderate hazard.
  - Clear area of personnel and move upwind.
  - Alert Emergency Responders and tell them location and nature of hazard.

Section 7 - HANDLING AND STORAGE

**PROCEDURE FOR HANDLING**

- The careful design and assembly of equipment is paramount to the control of mercaptan odors. Although careful planning reduces the chances for leaks developing in the system, it is important to be prepared to locate and stop small leaks promptly. It is recommended that a leak check be made prior to every run carried out under pressure in metal equipment with a mercaptan or hydrogen sulfide present.

An effective method to obtain a leak-free system involves two steps:

- Charge the system with nitrogen gas or other inert, nontoxic gas to a pressure at least as high as will be used in practice, and check for a drop in pressure with time on a suitable gauge. In some cases, it is advantageous to block off sections of the system to facilitate finding the leak. If any leaks are detected by using a foaming detergent solution, correct them and recheck.
- Recharge the system with hydrogen sulfide gas. Since hydrogen sulfide is very toxic, it is good practice to charge the system in steps of increasing pressure, until it is certain that no large leaks are present. Any remaining small leaks can be located quickly by examining the system with lead acetate paper. Dilution of the hydrogen sulfide with nitrogen can also be considered.

To control odors in mercaptan reactions in the laboratory: All reactions must be carried out in a hood or, in the case of pressure reactions, in a closed area equipped with an efficient exhaust fan. In the laboratory, the two basic types of reactions used are batch and continuous. Batch-type reactions at atmospheric pressure are generally conducted in glass equipment. If no significant quantity of a volatile mercaptan is present, the reaction can be carried out in a hood equipped with a charcoal bed in the exhaust line to absorb the mercaptan. In reactions where appreciable quantities of a volatile mercaptan are present, a vent gas line can be connected to two caustic scrubbers in series, with an empty trap inserted between the reaction and scrubbers to avoid reverse flow of caustic into the reaction. Continuous-type reactions often
include a continuous flow of volatile C1 to C4 mercaptans. In this case, the vented gases can be fed to an outside gas burner and stack for destruction of the odor by combustion.

A hood, equipped with a charcoal filter in the exhaust line, and a high linear air velocity (100 ft./min., minimum) is necessary for mercaptan reactions carried out in glass and certain small-scale reactions with stainless-steel. In reactions where relatively small amounts of mercaptans can escape, the charcoal bed can absorb the mercaptans and prevent the escape of odor to the outside atmosphere. However, in reactions with hydrogen sulfide or lower molecular weight mercaptans, e.g., C1-C4 mercaptans, the quantity of effluent gases is directed to an outside gas burner to convert the odorous compounds to acceptable combustion products, including CO2 and SO2.

A very familiar and successful method for containing the odors of mercaptan (primarily C1 and C6) in laboratory reactions and distillations is to connect the condenser vent to two caustic scrubbers in series with an empty trap between the system and the scrubbers to catch the caustic in the event of reverse flow. Gas bubblers fitted with sintered-glass dip tubes and charged with aqueous sodium hydroxide (5 to 20%) are commonly used. Frequently, a low flow of inert gas, e.g., nitrogen, is used to maintain a steady flow through the bubbler.

Sodium hypochlorite solution (3-10%) destroys the odor by converting the mercaptan predominantly to the corresponding sulfonic acid (sodium salt). A wash bottle with hypochlorite solution is very convenient for quickly eliminating or controlling the odor from small spills or when cleaning up glass equipment. A bath of this solution is also very useful. WARNING! Do not add this solution to a large quantity of concentrated mercaptan, since a violent reaction may occur.

A 30-40% aqueous solution of lead acetate trihydrate serves acts as a detector for methyl and ethyl mercaptan as well as hydrogen sulfide. A wash bottle of lead acetate solution is used to moisten a piece of filter paper or paper towel which is then held close to (no contact) the suspected leak. With hydrogen sulfide the paper turns black and with the two mercaptans a yellow color is obtained (high sensitivity).

A 30-40% aqueous solution of lead acetate trihydrate serves acts as a detector for methyl and ethyl mercaptan as well as hydrogen sulfide. A wash bottle of lead acetate solution is used to moisten a piece of filter paper or paper towel which is then held close to (no contact) the suspected leak. With hydrogen sulfide the paper turns black and with the two mercaptans a yellow color is obtained (high sensitivity).

Type of tubing found useful with mercaptans include: Teflon®, TFE, FEP, and PFA, Bev-a-line (IV or V), and 316 stainless steel. Bev-a-line tubing has a polyethylene liner cross-linked to an ethylene vinyl acetate shell, a useful temperature range of -60°C to +250°C, and is heat bondable. It is less expensive than TFE tubing and is convenient for flexible connections between glass and metal tubing lines. It is available from most laboratory supply houses. Copper and brass are unacceptable materials for handling mercaptans, because mercaptans are H2S highly corrosive to copper and brass. Care should be taken not to use valves and gauges with brass components.

Atofina Chemicals.

 Avoid all personal contact, including inhalation.

 Wear protective clothing when risk of exposure occurs.

 DO NOT allow clothing wet with material to stay in contact with skin.

RECOMMENDED STORAGE METHODS

- Metal can or drum
- Packing as recommended by manufacturer.

STORAGE REQUIREMENTS

- Store in original containers.
- Keep containers securely sealed.

### EXPOSURE CONTROLS

<table>
<thead>
<tr>
<th>Source</th>
<th>Material</th>
<th>TWA ppm</th>
<th>TWA mg/m³</th>
<th>STEL ppm</th>
<th>Peak ppm</th>
<th>Peak mg/m³</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>US NIOSH Recommended Exposure Limits (RELS)</td>
<td>n-dodecyl mercaptan (1-Dodecanethiol)</td>
<td>0.5</td>
<td>4.1</td>
<td>(Ceiling ([15-minute]])</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Canada - Nova Scotia Occupational Exposure Limits</td>
<td>n-dodecyl mercaptan (Dodecyl mercaptan)</td>
<td>0.1</td>
<td></td>
<td>TLV Basis: upper respiratory tract irritation</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Canada - Alberta Occupational Exposure Limits</td>
<td>n-dodecyl mercaptan (Dodecyl mercaptan)</td>
<td>0.1</td>
<td>0.8</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Canada - British Columbia Occupational Exposure Limits</td>
<td>n-dodecyl mercaptan (Dodecyl mercaptan)</td>
<td>0.1</td>
<td></td>
<td>S</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Canada - Ontario Occupational Exposure Limits</td>
<td>n-dodecyl mercaptan (Dodecyl mercaptan)</td>
<td>0.1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Canada - Saskatchewan Occupational Health and Safety Regulations - Contamination Limits</td>
<td>n-dodecyl mercaptan (Dodecyl mercaptan)</td>
<td>0.1</td>
<td>0.3</td>
<td>SEN</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Section 8 - EXPOSURE CONTROLS / PERSONAL PROTECTION
Canada - Prince Edward Island

Occupational Exposure Limits

<table>
<thead>
<tr>
<th>Substance</th>
<th>Concentration</th>
<th>TLV Basis: upper respiratory tract irritation</th>
</tr>
</thead>
<tbody>
<tr>
<td>n-dodecyl mercaptan (Dodecyl mercaptan)</td>
<td>0.1</td>
<td></td>
</tr>
</tbody>
</table>

US ACGIH Threshold Limit Values (TLV)

<table>
<thead>
<tr>
<th>Substance</th>
<th>Concentration</th>
<th>TLV Basis: upper respiratory tract irritation</th>
</tr>
</thead>
<tbody>
<tr>
<td>n-dodecyl mercaptan (Dodecyl mercaptan)</td>
<td>0.1</td>
<td></td>
</tr>
</tbody>
</table>

ENDOELTABLE

PERSONAL PROTECTION

RESPIRATOR
Type AB-P Filter of sufficient capacity
Consult your EHS staff for recommendations

EYE
- Safety glasses with side shields.
- Chemical goggles.

HANDS/FEET
- Wear chemical protective gloves, eg. PVC.

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.

OTHER
- Overalls.
- P.V.C. apron.
- Barrier cream.
- Skin cleansing cream.
- Eye wash unit.

ENGINEERING CONTROLS
- Local exhaust ventilation usually required. If risk of overexposure exists, wear an approved respirator.

Section 9 - PHYSICAL AND CHEMICAL PROPERTIES

PHYSICAL PROPERTIES

Liquid.
Mixes with water.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>State</td>
<td>Liquid</td>
<td>Molecular Weight</td>
</tr>
<tr>
<td>Melting Range (°F)</td>
<td>18.5</td>
<td>Viscosity</td>
</tr>
<tr>
<td>Boiling Range (°F)</td>
<td>289.4 (15 mm Hg)</td>
<td>Solubility in water (g/L)</td>
</tr>
<tr>
<td>Flash Point (°F)</td>
<td>260.6</td>
<td>pH (1% solution)</td>
</tr>
<tr>
<td>Decomposition Temp (°F)</td>
<td>&gt;662</td>
<td>pH (as supplied)</td>
</tr>
<tr>
<td>Autoignition Temp (°F)</td>
<td>Not available.</td>
<td>Vapour Pressure (mmHG)</td>
</tr>
<tr>
<td>Upper Explosive Limit (%)</td>
<td>Not available.</td>
<td>Specific Gravity (water=1)</td>
</tr>
<tr>
<td>Lower Explosive Limit (%)</td>
<td>Not available.</td>
<td>Relative Vapor Density (air=1)</td>
</tr>
</tbody>
</table>

5 of 8
Volatile Component (%vol) | Not available | Evaporation Rate | Not available
--- | --- | --- | ---

**APPEARANCE**

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**Section 10 - CHEMICAL STABILITY**

**CONDITIONS CONTRIBUTING TO INSTABILITY**
- Presence of incompatible materials.
- Product is considered stable.

**STORAGE INCOMPATIBILITY**
- Avoid reaction with oxidizing agents, bases and strong reducing agents.
- Avoid alkali metals.

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

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**Section 11 - TOXICOLOGICAL INFORMATION**

**N-DODECYL MERCAPTAN**

**TOXICITY AND IRRITATION**
- unless otherwise specified data extracted from RTECS - Register of Toxic Effects of Chemical Substances.

<table>
<thead>
<tr>
<th>TOXICITY</th>
<th>IRRITATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oral (mouse) LD50: &gt;5000 mg/kg *</td>
<td>Skin (unspec): irritating *</td>
</tr>
<tr>
<td>Oral (mouse) LC50: 4225 mg/kg **</td>
<td>Eye (unspec): irritating *</td>
</tr>
</tbody>
</table>

* [Atochem] ** [Patty's]

- Asthma-like symptoms may continue for months or even years after exposure to the material ceases. This may be due to a non-allergic 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.

- Allergic reactions involving the respiratory tract are usually due to interactions between IgE antibodies and allergens and occur rapidly. Allergic potential of the allergen and period of exposure often determine the severity of symptoms.

Attention should be paid to atopic diathesis, characterized by increased susceptibility to nasal inflammation, asthma and eczema.

Exogenous allergic alveolitis is induced essentially by allergen specific immune-complexes of the IgG type; cell-mediated reactions (T lymphocytes) may be involved. Such allergy is of the delayed type with onset up to four hours following exposure. Contact allergies quickly manifest themselves as contact eczema, more rarely as urticaria or Quincke's edema. The pathogenesis of contact eczema involves a cell-mediated (T lymphocytes) immune reaction of the delayed type.

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**Section 12 - ECOLOGICAL INFORMATION**

This material and its container must be disposed of as hazardous waste.

**Ecotoxicity**

<table>
<thead>
<tr>
<th>Ingredient</th>
<th>Persistence: Water/Soil</th>
<th>Persistence: Air</th>
<th>Bioaccumulation</th>
<th>Mobility</th>
</tr>
</thead>
<tbody>
<tr>
<td>n-dodecyl mercaptan</td>
<td>LOW</td>
<td>LOW</td>
<td>LOW</td>
<td>LOW</td>
</tr>
</tbody>
</table>

---

**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.

Section 14 - TRANSPORTATION INFORMATION

Air Transport IATA:
ICAO/IATA Class: 9 ICAO/IATA Subrisk: None
UN/ID Number: 3334 Packing Group: -
Special provisions: A27
Cargo Only
Packing Instructions: 906 Maximum Qty/Pack: 220 L
Passenger and Cargo Passenger and Cargo
Packing Instructions: 906 Maximum Qty/Pack: 100 L
Passenger and Cargo Limited Quantity Passenger and Cargo Limited Quantity
Packing Instructions: - Maximum Qty/Pack: -
Shipping Name: AVIATION REGULATED LIQUID, N.O.S. *
†(CONTAINS N-DODECYL MERCAPTAN)
NOT REGULATED FOR TRANSPORT OF DANGEROUS GOODS: DOT, IMDG

Section 15 - REGULATORY INFORMATION

REGULATIONS
n-dodecyl mercaptan (CAS: 112-55-0) is found on the following regulatory lists;

Section 16 - OTHER INFORMATION

LIMITED EVIDENCE
- Inhalation may produce health damage*.
- Cumulative effects may result following exposure*.
* (limited evidence).

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Classification of the preparation 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.

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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