

1-(3-Chloropropyl)theobromine: sc-287000



The Power to Question

MATERIAL SAFETY DATA SHEET

| HAZARD WARNINGS | RISK PHRASES | PROTECTIVE CLOTHING |
|-----------------|--------------------------------------|---------------------|
| | Harmful compound, minimize exposure. | |

Section I. Chemical Product and Company Identification

| | | | |
|------------------|--|-----------|---|
| Chemical Name | 1-(3-Chloropropyl)theobromine | Supplier | Santa Cruz Biotechnology, Inc. 2145 Delaware Avenue Santa Cruz, California 95060 800.457.3801 or 831.457.3800 |
| Catalog Number | sc-287000 | | |
| CAS Number | 74409-52-2 | | |
| Chemical Formula | C10H13ClN4O2 | Emergency | ChemWatch Within the US & Canada: 877-715-9305 Outside the US & Canada: +800 2436 2255 (1-800-CHEMCALL) or call +613 9573 3112 |
| Synonym | 1-(3-Chloropropyl)-3,7-dihydro-3,7-dimethyl-1H-purine-2,6-dione; 1-(3-Chloropropyl)-3,7-dimethylxanthine | | |

Section II. Composition and Information on Ingredients

| Chemical Name | CAS Number | Percent (%) | TLV/PEL | Toxicology Data |
|-------------------------------|------------|---------------------|----------------|-----------------|
| 1-(3-Chloropropyl)theobromine | 74409-52-2 | Min. 95.0 (HPLC, T) | Not available. | Not available. |

Section III. Hazards Identification


| | |
|------------------------|--|
| Acute Health Effects | Harmful if ingested or inhaled. Minimize exposure to this material. Severe overexposure can result in injury or death. Follow safe industrial hygiene practices and always wear proper protective equipment when handling this compound. |
| Chronic Health Effects | CARCINOGENIC EFFECTS : Not available. MUTAGENIC EFFECTS : Not available. TERATOGENIC EFFECTS : Not available. DEVELOPMENTAL TOXICITY : Not available. Repeated or prolonged exposure to this compound is not known to aggravate existing medical conditions. |

Section IV. First Aid Measures

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|--------------|---|
| Eye Contact | Check for and remove any contact lenses. In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. Get medical attention. |
| Skin Contact | In case of contact, immediately flush skin with plenty of water. Remove contaminated clothing and shoes. Wash clothing before reuse. Thoroughly clean shoes before reuse. Get medical attention. |
| Inhalation | If the victim is not breathing, perform mouth-to-mouth resuscitation. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, oxygen can be administered. Seek medical attention if respiration problems do not improve. |
| Ingestion | INDUCE VOMITING by sticking finger in throat. Lower the head so that the vomit will not reenter the mouth and throat. Loosen tight clothing such as a collar, tie, belt or waistband. If the victim is not breathing, perform mouth-to-mouth resuscitation. Examine the lips and mouth to ascertain whether the tissues are damaged, a possible indication that the toxic material was ingested; the absence of such signs, however, is not conclusive. |

Section V. Fire and Explosion Data

| | | | |
|--------------------------------------|--|------------------|----------------|
| Flammability | May be combustible at high temperature. | Auto-Ignition | Not available. |
| Flash Points | Not available. | Flammable Limits | Not available. |
| Combustion Products | These products are toxic carbon oxides (CO, CO ₂), nitrogen oxides (NO, NO ₂), halogenated compounds. WARNING: Highly toxic HCl gas is produced during combustion. | | |
| Fire Hazards | Not available. | | |
| Explosion Hazards | Risks of explosion of the product in presence of mechanical impact: Not available. Risks of explosion of the product in presence of static discharge: Not available. | | |
| Fire Fighting Media and Instructions | SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use water spray, fog or foam. DO NOT use water jet. Consult with local fire authorities before attempting large scale fire-fighting operations. | | |

| Section VI. Accidental Release Measures | | | |
|---|---|-----------------------|--------------------------|
| Spill Cleanup Instructions | Harmful material. Use a shovel to put the material into a convenient waste disposal container. Consult federal, state, and/or local authorities for assistance on disposal. | | |
| Section VII. Handling and Storage | | | |
| Handling and Storage Information | HARMFUL. Keep away from heat. Mechanical exhaust required. When not in use, tightly seal the container and store in a dry, cool place. Avoid excessive heat and light. Do not breathe dust. Always store away from incompatible compounds such as oxidizing agents. | | |
| Section VIII. Exposure Controls/Personal Protection | | | |
| Engineering Controls | Use process enclosures, local exhaust ventilation, or other engineering controls to keep airborne levels below recommended exposure limits. If user operations generate dust, fume or mist, use ventilation to keep exposure to airborne contaminants below the exposure limit. | | |
| Personal Protection | Splash goggles. Lab coat. Dust respirator. Boots. Gloves. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product. Be sure to use a MSHA/NIOSH approved respirator or equivalent. <div></div> | | |
| Exposure Limits | Not available. | | |
| Section IX. Physical and Chemical Properties | | | |
| Physical state @ 20°C | Solid. | Solubility | Soluble in hot methanol. |
| Specific Gravity | Not available. | | |
| Molecular Weight | 256.69 | Partition Coefficient | Not available. |
| Boiling Point | Not available. | Vapor Pressure | Not applicable. |
| Melting Point | 144 to 148 °C (291.2 to 298.4 °F) | Vapor Density | Not available. |
| Refractive Index | Not available. | Volatility | Not available. |
| Critical Temperature | Not available. | Odor | Not available. |
| Viscosity | Not available. | Taste | Not available. |
| Section X. Stability and Reactivity Data | | | |
| Stability | This material is stable if stored under proper conditions. (See Section VII for instructions) | | |
| Conditions of Instability | Avoid excessive heat and light. | | |
| Incompatibilities | Reactive with oxidizing agents. | | |
| Section XI. Toxicological Information | | | |
| RTECS Number | Not available. | | |
| Routes of Exposure | Eye Contact. Ingestion. Inhalation. | | |
| Toxicity Data | Not available. | | |
| Chronic Toxic Effects | CARCINOGENIC EFFECTS : Not available. MUTAGENIC EFFECTS : Not available. TERATOGENIC EFFECTS : Not available. DEVELOPMENTAL TOXICITY : Not available. Repeated or prolonged exposure to this compound is not known to aggravate existing medical conditions. | | |
| Acute Toxic Effects | Harmful if ingested or inhaled. Minimize exposure to this material. Severe overexposure can result in injury or death. Follow safe industrial hygiene practices and always wear proper protective equipment when handling this compound. | | |
| Section XII. Ecological Information | | | |
| Ecotoxicity | Not available. | | |
| Environmental Fate | Not available. | | |

Section XIII. Disposal Considerations

Waste Disposal

Recycle to process, if possible. Consult your local regional authorities. You may be able to dissolve or mix material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber system. Observe all federal, state and local regulations when disposing of the substance.

Section XIV. Transport Information

DOT Classification

Not a DOT controlled material (United States).

PIN Number

Not applicable.

Proper Shipping Name

Not applicable.

Packing Group (PG)

Not applicable.

DOT Pictograms

**Section XV. Other Regulatory Information and Pictograms**TSCA Chemical Inventory
(EPA)

This product is **NOT** on the EPA Toxic Substances Control Act (TSCA) inventory. The following notices are required by 40 CFR 720.36 (C) for those products not on the inventory list:

(i) These products are supplied solely for use in research and development by or under the supervision of a technically qualified individual as defined in 40 CFR 720.0 et sec.
(ii) The health risks of these products have not been fully determined. Any information that is or becomes available will be supplied on an MSDS sheet.

WHMIS Classification
(Canada)

Not available.

EINECS Number (EEC)

Not available.

EEC Risk Statements

R20/21/22- Harmful by inhalation, in contact with skin and if swallowed.

Japanese Regulatory Data

Not available.

Section XVI. Other Information

Notice to Reader:

The above information is believed to be correct but does not purport to be complete and should be used only as a guide. The burden of safe use of this material rests entirely with the user.