

# Material Safety Data Sheet

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

## Section I. Chemical Product and Company Identification

|                  |   |                                 |   |
|------------------|---|---------------------------------|---|
| Chemical Name    | <b>Theobromine</b>  |                                 |   |
| Catalog Number   | T0178   | Supplier                        | TGI America<br>9211 N. Harborage St.<br>Portland OR<br>1-800-423-8616                     |
| Synonym          | 3,7-Dimethylxanthine  |                                 |   |
| Chemical Formula | C <sub>7</sub> H <sub>8</sub> N <sub>4</sub> O <sub>2</sub> |                                 |   |
| CAS Number       | 83-67-0   | In case of<br>Emergency<br>Call | <b>Chemtrec®</b><br><b>(800) 424-9300 (U.S.)</b><br><b>(703) 527-3887 (International)</b> |

## Section II. Composition and Information on Ingredients

| Chemical Name | CAS Number | Percent (%)                | TLV/PEL        | Toxicology Data  |
|---------------|------------|----------------------------|----------------|--|
| Theobromine   | 83-67-0    | Min. 98.0%<br>(HPLC, Tit.) | Not available. | Rat LD <sub>50</sub> (oral) 1265 mg/kg<br>Mouse LD <sub>50</sub> (oral) 837 mg/kg<br>Mouse LD <sub>50</sub> (subcutaneous) 530 mg/kg |

## 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 | <p><b>CARCINOGENIC EFFECTS</b> : Not available.</p> <p><b>MUTAGENIC EFFECTS</b> : Not available.</p> <p><b>TERATOGENIC EFFECTS</b> : Not available.</p> <p><b>DEVELOPMENTAL TOXICITY: REPRODUCTIVE EFFECTS</b><br/>Rat TDLo Oral; 7500 mg/kg; male 49 days prior to mating</p> <p><b>TOXIC EFFECTS</b><br/>Paternal Effects - Testes, epididymis, sperm duct<br/>TDLo Oral; 17640 mg/kg; male 49 days prior to mating</p> <p><b>TOXIC EFFECTS</b><br/>Effects on Fertility - Male fertility index (e.g., number males impregnating females per number males exposed to fertile nonpregnant females)<br/>Mouse TDLo Intraperitoneal; 500 mg/kg; female 13 days of pregnancy</p> <p><b>TOXIC EFFECTS</b><br/>Effects on Embryo or Fetus - Tetotoxicity (except death, e.g., stunted fetus)<br/>Specific Developmental Abnormalities - Craniofacial (including nose and tongue)<br/>Specific Developmental Abnormalities - Musculoskeletal system</p> <p>Repeated or prolonged exposure to this compound is not known to aggravate existing medical conditions.</p> |

## Section IV. First Aid Measures

|              |   |
|--------------|---|
| 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. |

| <b>Section V. Fire and Explosion Data</b> |  |                  |                |
|---|--|------------------|----------------|
| 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 <sub>2</sub> ), nitrogen oxides (NO, NO <sub>2</sub> ).   |                  |                |
| Fire Hazards                              | Not available.   |                  |                |
| Explosion Hazards                         | Risks of explosion of the product in presence of mechanical impact: Not available.<br>Risks of explosion of the product in presence of static discharge: Not available.                                |                  |                |
| Fire Fighting Media and Instructions      | SMALL FIRE: Use DRY chemical powder.<br>LARGE FIRE: Use water spray, fog or foam. DO NOT use water jet.<br>Consult with local fire authorities before attempting large scale fire-fighting operations. |                  |                |

| <b>Section VI. Accidental Release Measures</b> |  |
|--|--|
| Spill Cleanup Instructions                     | Harmful Material.<br>Use a shovel to put the material into a convenient waste disposal container. Finish cleaning the spill by rinsing any contaminated surfaces with copious amounts of water. Consult federal, state, and/or local authorities for assistance on disposal. |

| <b>Section VII. Handling and Storage</b> |  |
|--|--|
| 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.<br>Always store away from incompatible compounds such as oxidizing agents. |

| <b>Section VIII. Exposure Controls/Personal Protection</b> |   |
|--|---|
| 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.  |
|  |   |
| Exposure Limits  | Not available.  |

| <b>Section IX. Physical and Chemical Properties</b> |                        |                       |  |
|---|------------------------|-----------------------|--|
| Physical state @ 20°C                               | Solid. (White Powder.) | Solubility            | Soluble in sodium hydroxide solution, alcohol, fixed alkali hydroxides, concentrated acids, water (1g dissolves in 2000 ml water, 150 ml boiling water). Slightly soluble in ammonia. Insoluble in benzene, ether, chloroform, carbon tetrachloride. |
| Specific Gravity                                    | Not available.         |                       |  |
| Molecular Weight                                    | 180.16                 | Partition Coefficient | Not available.   |
| Boiling Point                                       | Not available.         | Vapor Pressure        | Not applicable.  |
| Melting Point                                       | 345 °C (653 °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.   |

| <b>Section X. Stability and Reactivity Data</b> |   |
|---|---|
| Stability                                       | This material is stable if stored under proper conditions. (See Section VII for instructions) |
| Conditions of Instability                       | Avoid excessive heat and light.   |
| Incompatibilities                               | Highly reactive with oxidizing agents.  |

**Section XI. Toxicological Information**

|                       |   |
|-----------------------|---|
| RTECS Number          | XH2275000   |
| Routes of Exposure    | Eye Contact. Ingestion. Inhalation.   |
| Toxicity Data         | Rat LD <sub>50</sub> (oral) 1265 mg/kg<br>Mouse LD <sub>50</sub> (oral) 837 mg/kg<br>Mouse LD <sub>50</sub> (subcutaneous) 530 mg/kg  |
| Chronic Toxic Effects | <b>CARCINOGENIC EFFECTS</b> : Not available.<br><b>MUTAGENIC EFFECTS</b> : Not available.<br><b>TERATOGENIC EFFECTS</b> : Not available.<br><b>DEVELOPMENTAL TOXICITY: REPRODUCTIVE EFFECTS</b><br>Rat TDLo Oral; 7500 mg/kg; male 49 days prior to mating<br><b>TOXIC EFFECTS</b><br>Paternal Effects - Testes, epididymis, sperm duct<br>TDLo Oral; 17640 mg/kg; male 49 days prior to mating<br><b>TOXIC EFFECTS</b><br>Effects on Fertility - Male fertility index (e.g., number males impregnating females per number males exposed to fertile nonpregnant females)<br>Mouse TDLo Intraperitoneal; 500 mg/kg; female 13 days of pregnancy<br><b>TOXIC EFFECTS</b><br>Effects on Embryo or Fetus - Tetotoxicity (except death, e.g., stunted fetus)<br>Specific Developmental Abnormalities - Craniofacial (including nose and tongue)<br>Specific Developmental Abnormalities - Musculoskeletal system<br>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 | Theobromine's former production and use as a diuretic, bronchodilator, cardiogenic as well as being an alkaloid found in cocoa and chocolate products may result in its release to the environment through various waste streams. Theobromine is the principal alkaloid of the cacao bean and occurs in fresh tea leaves. If released to air, an estimated vapor pressure of 8.9X10 <sup>-10</sup> mm Hg at 25 deg C indicates theobromine will exist solely in the particulate phase in the ambient atmosphere. Particulate-phase theobromine will be removed from the atmosphere by wet and dry deposition. Theobromine does not absorb light at wavelengths >290 nm and therefore is not expected to be susceptible to direct photolysis by sunlight. If released to soil, theobromine is expected to have very high mobility based upon an estimated Koc of 9. Volatilization from moist soil surfaces is not expected to be an important fate process based upon an estimated Henry's Law constant of 1.6X10 <sup>-11</sup> atm-cu m/mole. The pKa of theobromine is 9.90, indicating that this compound will partially exist in the protonated form in the environment and cations generally adsorb more strongly to organic carbon and clay than their neutral counterparts. Theobromine is readily biodegradable following acclimation, suggesting that biodegradation may be an important environmental fate process. If released into water, theobromine is not expected to adsorb to suspended solids and sediment based upon the estimated Koc. Volatilization from water surfaces is not expected to be an important fate process based upon this compound's estimated Henry's Law constant. A pKa of 9.90 indicates theobromine will partially exist in the ionized form at pH values of 5 to 9 and therefore volatilization from water surfaces is not expected to be an important environmental fate process. An estimated BCF of 3 suggests the potential for bioconcentration in aquatic organisms is low. Hydrolysis is not expected to be an important environmental fate process since this compound lacks functional groups that hydrolyze under environmental conditions. Occupational exposure to theobromine may occur through inhalation and dermal contact with this compound at workplaces where theobromine is produced. Monitoring data indicate that the general population may be exposed to theobromine via ingestion of food and dermal contact with this compound and other consumer products containing theobromine. Exposure among the general population may have occurred to those administered the drug (a diuretic). |

**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 compound is <b>ON</b> the EPA Toxic Substances Control Act (TSCA) inventory list. |
| WHMIS Classification (Canada) | On DSL.  |
| EINECS Number (EEC)           | 201-494-2  |
| EEC Risk Statements           | R20/21/22- Harmful by inhalation, in contact with skin and if swallowed.               |
| Japanese Regulatory Data      | ENCS No. (9)-847   |

**Section XVI. Other Information**

**Version 1.0**  
**Validated on 6/29/2007.**  
**Printed 6/29/2007.**

**Notice to Reader**

TCI laboratory chemicals are for research purposes only and are NOT intended for use as drugs, food additives, households, or pesticides. The information herein is believed to be correct, but does not claim to be all inclusive and should be used only as a guide. Neither the above named supplier nor any of its subsidiaries assumes any liability whatsoever for the accuracy or completeness of the information contained herein. Final determination of suitability of any material is the sole responsibility of the user. All chemical reagents must be handled with the recognition that their chemical, physiological, toxicological, and hazardous properties have not been fully investigated or determined. All chemical reagents should be handled only by individuals who are familiar with their potential hazards and who have been fully trained in proper safety, laboratory, and chemical handling procedures. Although certain hazards are described herein, we can not guarantee that these are the only hazards which exist. Our MSDS sheets are based only on data available at the time of shipping and are subject to change without notice as new information is obtained. Avoid long storage periods since the product is subject to degradation with age and may become more dangerous or hazardous. It is the responsibility of the user to request updated MSDS sheets for products that are stored for extended periods. Disposal of unused product must be undertaken by qualified personnel who are knowledgeable in all applicable regulations and follow all pertinent safety precautions including the use of appropriate protective equipment (e.g. protective goggles, protective clothing, breathing equipment, facial mask, fume hood). For proper handling and disposal, always comply with federal, state, and local regulations.

Printed 6/29/2007.