

# Material Safety Data Sheet

| HAZARD WARNINGS                                                                   | RISK PHRASES                                                                   | PROTECTIVE CLOTHING                                                                                                                                                                                                                                                                                                                             |
|-----------------------------------------------------------------------------------|--------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|  | Toxic compound, do not ingest or inhale. Avoid all contact with this material. |     |

## Section I. Chemical Product and Company Identification

|                  |                                                             |                                 |                                                                                          |
|------------------|-------------------------------------------------------------|---------------------------------|------------------------------------------------------------------------------------------|
| Chemical Name    | <b>Theophylline</b>                                         |                                 |                                                                                          |
| Catalog Number   | T0179                                                       | Supplier                        | TCI America<br>9211 N. Harbortgate St.<br>Portland OR<br>1-800-423-8616                  |
| Synonym          | 1,3-Dimethylxanthine                                        |                                 |                                                                                          |
| Chemical Formula | C <sub>7</sub> H <sub>8</sub> N <sub>4</sub> O <sub>2</sub> |                                 |                                                                                          |
| CAS Number       | 58-55-9                                                     | In case of<br>Emergency<br>Call | <b>Chemtec®</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                                                                                                                            |
|---------------|------------|------------------------|----------------|--------------------------------------------------------------------------------------------------------------------------------------------|
| Theophylline  | 58-55-9    | Min. 98.0<br>(HPLC, T) | Not available. | Rat LD <sub>50</sub> (oral) 225mg/kg<br>Rat LD <sub>50</sub> (intravenous) 240mg/kg<br>Mouse LD <sub>50</sub> (intraperitoneal)<br>70mg/kg |

## Section III. Hazards Identification

|                        |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
|------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Acute Health Effects   | Toxic if ingested or inhaled. Avoid prolonged contact with this material. Overexposure may result in serious illness or death. Follow safe industrial hygiene practices and always wear proper protective equipment when handling this compound.                                                                                                                                                                                                                                                                                                               |
| Chronic Health 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</b> : Reproductive: rat (oral) 75335mg/kg duration: male 67 days prior to mating.<br>Paternal effects- Spermatogenesis.<br>rat (oral) 10050mg/kg duration: male 67 days prior to mating.<br>Paternal effects- Testes, epidymis, sperm duct.<br>Repeated exposure to an highly toxic material may produce general deterioration of health by an accumulation in one or many human organs. |

## Section IV. First Aid Measures

|              |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
|--------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Eye Contact  | Check for and remove any contact lenses. IMMEDIATELY flush eyes with running water for at least 15 minutes, keeping eyelids open. WARM water MUST be used. DO NOT use an eye ointment. Flush eyes with running water for a minimum of 15 minutes, occasionally lifting the upper and lower eyelids. Seek medical attention. Treat symptomatically and supportively.                                                                                                                                                                                                       |
| Skin Contact | After contact with skin, wash immediately with plenty of water. WARM water MUST be used. Gently and thoroughly wash the contaminated skin with running water and non-abrasive soap. Be particularly careful to clean folds, crevices, creases and groin. Cover the irritated skin with an emollient. Seek medical attention. Treat symptomatically and supportively. Wash any contaminated clothing before reusing.                                                                                                                                                       |
| Inhalation   | If the victim is not breathing, perform artificial respiration. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, oxygen can be administered. Seek medical attention. Treat symptomatically and supportively.                                                                                                                                                                                                                                                                                                                    |
| 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, administer artificial respiration. 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. Seek immediate medical attention and, if possible, show the chemical label. Treat symptomatically and supportively. |

## Section V. Fire and Explosion Data

|                                      |                                                                                                                                                                                                                                                     |                  |                |
|--------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------|----------------|
| Flammability                         | Combustible.                                                                                                                                                                                                                                        | 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                         | No specific information is available regarding the flammability of this compound in the presence of various materials.                                                                                                                              |                  |                |
| 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.<br>No additional information is available regarding the risks of explosion. |                  |                |
| Fire Fighting Media and Instructions | SMALL FIRE: Use DRY chemicals, CO <sub>2</sub> , water spray or foam.<br>LARGE FIRE: Use water spray, fog or foam. DO NOT use water jet.                                                                                                            |                  |                |

Continued on Next Page

Emergency phone number (800) 424-9300

**Section VI. Accidental Release Measures****Spill Cleanup  
Instructions**

Toxic solid.  
Stop leak if without risk. DO NOT get water inside container. DO NOT touch spilled material. Use water spray to reduce vapors. Prevent entry into sewers, basements or confined areas; dike if needed. Eliminate all sources of ignition. Consult federal, state, and/or local authorities for assistance on disposal. 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.

**Section VII. Handling and Storage****Handling and Storage  
Information**

TOXIC. Handle with caution and minimize exposure. Keep away from heat and sources of ignition. 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 ingest. DO NOT breathe dust. In case of insufficient ventilation, wear suitable respiratory equipment. If ingested, seek medical advice immediately and show the container or the label. Treat symptomatically and supportively. Avoid contact with skin and eyes.  
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. A MSHA/NIOSH approved respirator must be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

**Exposure Limits**

Not available.

**Section IX. Physical and Chemical Properties****Physical state @ 20°C**

White crystalline powder.

**Solubility**

Soluble in hot water, alkali hydroxides, ammonia, dilute hydrochloric acid or nitric acid.

**Specific Gravity**

Not available.

**Molecular Weight**

180.17

**Partition Coefficient**

Not available.

**Boiling Point**

Not available.

**Vapor Pressure**

Not available.

**Melting Point**

Not available.

**Vapor Density**

Not available.

**Refractive Index**

Not available.

**Volatility**

Not available.

**Critical Temperature**

Not available.

**Odor**

Odorless.

**Viscosity**

Not available.

**Taste**

Bitter taste.

**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**

XH3850000

**Routes of Exposure**

Eye contact. Inhalation. Ingestion.

**Toxicity Data**

Rat LD<sub>50</sub> (oral) 225mg/kg  
Rat LD<sub>Lo</sub> (intravenous) 240mg/kg  
Mouse LD<sub>50</sub> (intraperitoneal) 70mg/kg

**Chronic Toxic Effects**

**CARCINOGENIC EFFECTS** : Not available.  
**MUTAGENIC EFFECTS** : Not available.  
**TERATOGENIC EFFECTS** : Not available.  
**DEVELOPMENTAL TOXICITY**: Reproductive: rat (oral) 75335mg/kg duration: male 67 days prior to mating.  
Paternal effects- Spermatogenesis.  
rat (oral) 10050mg/kg duration: male 67 days prior to mating.  
Paternal effects- Testes, epidymis, sperm duct.  
Repeated exposure to an highly toxic material may produce general deterioration of health by an accumulation in one or many human organs.

**Acute Toxic Effects**

Toxic if ingested or inhaled. Avoid prolonged contact with this material. Overexposure may result in serious illness 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 | The release of theophylline in the environment is expected to occur during production of the compound and during discharge of effluents from hospitals using the medicine. The presence of suitable chromophoric group suggests that theophylline may absorb sunlight and may photodegrade, but the rate of photodegradation under environmental conditions remains unknown. Screening tests for biodegradability indicate that theophylline may be biodegradable in soil and water. The adsorption of theophylline to suspended solids and sediments in water and to soil should be unimportant. Based on estimated Henry's Law constant, the volatilization of theophylline from water should not occur. The estimated bioconcentration factor indicates that bioconcentration of theophylline in aquatic organisms should not be important. If present in the atmosphere in the vapor phase, the reaction of theophylline with photochemically produced hydroxyl radicals may be important (estimated half-life 2.5 hrs). The most probable route of exposure to theophylline is expected to be ingestion for patients using the medication and probably inhalation of powder by workers during production/formulation of the medicine. (SRC) |

**Section XIII. Disposal Considerations**

|                |                                                                                                                                                                                                                                                                                                                              |
|----------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Waste Disposal | Recycle to process, if possible. Consult your local or 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 this 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) | WHMIS CLASS D-1B: Material causing immediate and serious toxic effects (TOXIC).        |
| EINECS Number (EEC)           | 200-385-7                                                                              |
| EEC Risk Statements           | R23/24/25- Toxic by inhalation, in contact with skin and if swallowed.                 |
| Japanese Regulatory Data      | Not available.                                                                         |

**Section XVI. Other Information**

**Version 1.0**  
**Validated on 2/17/1998.**  
**Printed 2/11/2011.**

**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.