

Material Safety Data Sheet (MSDS)

Theobromine

Revision Date: 06-02-2026

Version: 1.0

Section 1: Product Identification

- **Product Name:** Theobromine
- **Chemical Formula:** C₇H₈N₄O₂
- **CAS No:** 83-67-0
- **Synonyms:** 2,6-Dihydroxy-3,7-Dimethylpurine, 3,7-Dihydro-3,7-Dimethyl-1H-Purine-2,6-Dione
- **Recommended Use:** Stimulant used in pharmaceutical research and as a natural alkaloid in cacao products; also used as a chemical intermediate

Section 2: Hazards Identification

- **Classification (GHS):** Flammable liquids; Acute toxicity, Oral; Skin irritation; Eye irritation.
- **Signal Word:** Warning
- **Hazard Statements:**
 - Harmful if swallowed
 - Causes skin irritation and serious eye irritation
 - Combustible liquid
 - Keep away from heat/sparks/open flames. No smoking
 - Wear protective gloves/eye protection
 - **IF ON SKIN or IN EYES:** Rinse cautiously with water; seek medical advice if irritation persists

Section 3: Composition / Information on Ingredients

- **Concentration:** 99–99.5%
-

Section 4: First Aid Measures

- **Inhalation:** Remove to fresh air. If symptoms develop, seek medical attention.
 - **Skin Contact:** Wash with plenty of soap and water. Remove contaminated clothing. Seek medical advice if irritation persists.
 - **Eye Contact:** Rinse cautiously with water for several minutes. Remove contact lenses if present. Continue rinsing. Seek medical attention if irritation persists.
 - **Ingestion:** Rinse mouth. Do NOT induce vomiting. Seek medical advice if feeling unwell.
-

Section 5: Fire-Fighting Measures

- **Suitable Extinguishing Media:** Dry chemical, foam, carbon dioxide water spray.
 - **Specific Hazards:** Combustible liquid; emits toxic fumes of carbon oxides under fire conditions.
 - **Protective Equipment:** Firefighters should wear self-contained breathing apparatus and protective clothing.
-

Section 6: Accidental Release Measures

- **Personal Precautions:** Use personal protective equipment. Avoid breathing vapors. Ensure adequate ventilation. Eliminate ignition sources.
- **Environmental Precautions:** Prevent entry into drains and waterways.



- **Cleanup Methods:** Absorb with inert material. Collect in suitable container for disposal.
-

Section 7: Handling and Storage

- **Handling:** Avoid inhalation of vapors and contact with skin/eyes. Use with adequate ventilation. Keep away from ignition sources.
 - **Storage:** Keep container tightly closed. Store in a cool, dry, well-ventilated place away from heat and oxidizing agents.
-

Section 8: Exposure Controls / Personal Protection

- **Exposure Limits:** ACGIH TLV 50 ppm 205 mg/m³ TWA; OSHA PEL not established.
 - **Engineering Controls:** Provide adequate ventilation and local exhaust if needed.
 - **Personal Protective Equipment:** Chemical-resistant gloves, safety goggles, protective clothing. Respirator if ventilation is inadequate.
-

Section 9: Physical and Chemical Properties

- **Appearance:** White crystalline powder
 - **Boiling Point:** 400 °C
 - **Flash Point:** 210 °C
 - **Solubility:** Very slightly soluble in water; 0.06 g/100 mL at 25 °C
 - **Molecular Weight:** 180.17 g/mol
-

Section 10: Stability and Reactivity

- **Stability:** Stable under normal conditions.
- **Incompatible Materials:** Strong oxidizing agents.



- **Hazardous Decomposition Products:** Carbon oxides under fire conditions.
-

Section 11: Toxicological Information

- **Routes of Exposure:** Inhalation, ingestion, skin and eye contact.
 - **Acute Effects:** Harmful if swallowed; causes skin and eye irritation; may cause respiratory irritation.
 - **Chronic Effects:** Prolonged or repeated exposure may cause dermatitis and liver/kidney effects.
-

Section 12: Ecological Information

- **Ecotoxicity:** May be harmful to aquatic life in high concentrations.
 - **Persistence and Degradability:** Expected to be biodegradable.
 - **Bioaccumulative Potential:** Low to moderate potential.
-

Section 13: Disposal Considerations

- Dispose of contents/container in accordance with local/regional/national regulations. Do not release into the environment.
-

Section 14: Transport Information

- **Proper Shipping Name:** Theobromine
-

Section 15: Regulatory Information

- Complies with Indian chemical safety regulations and listed under international chemical inventories.
- Classified as hazardous substance as per GHS.



Section 16: Other Information

- **Disclaimer:** The above information is believed to be correct but does not claim to be exhaustive. Users are responsible for verifying suitability under actual conditions of use. **Triveni chemicals** disclaim any liability for damage resulting from handling or contact.

