



# TCI AMERICA

## SAFETY DATA SHEET

Revision number: 1  
Revision date: 07/06/2018

### 1. IDENTIFICATION

**Product name:** Theobromine  
**Product code:** T0178

**Product use:** For laboratory research purposes.  
**Restrictions on use:** Not for drug or household use.

Company:  
TCI America  
9211 N. Harborside Street  
Portland, OR 97203 U.S.A.  
Telephone:  
+1-800-423-8616 / +1-503-283-1681  
Fax:  
+1-888-520-1075 / +1-503-283-1987  
e-mail:  
sales-US@TCIchemicals.com  
www.TCIchemicals.com

**Emergency telephone number:**  
Chemical Emergencies:  
TCI America (8:00am - 5:00pm) PST  
+1-503-286-7624  
Transportation Emergencies:  
Chemtrec 24-Hour  
+1-800-424-9300 (U.S.A.)  
+1-703-527-3887 (International)  
**Responsible department:**  
TCI America  
Environmental Health Safety and Security  
+1- 503-286-7624

### 2. HAZARD(S) IDENTIFICATION

**OSHA Haz Com: CFR 1910.1200:** Acute Toxicity - Oral [Category 4]  
**WHMIS 2015:**

**Signal word:** Warning!

**Hazard Statement(s):** Harmful if swallowed

**Pictogram(s) or Symbol(s):**



**Precautionary Statement(s):**  
[Prevention]  
[Response]  
[Disposal]

Do not eat, drink or smoke when using this product. Wash hands and face thoroughly after handling.  
If swallowed: Call a poison center or doctor if you feel unwell. Rinse mouth.  
Dispose of contents and container in accordance with local, regional, national regulations (e.g. US: 40 CFR Part 261, EU:91/156/EEC, JP: Waste Disposal and Cleaning Act, etc.).

**Hazards not otherwise classified:** None.  
**[HNOC]**

### 3. COMPOSITION/INFORMATION ON INGREDIENTS

**Substance/mixture:** Substance  
**Components:** Theobromine  
**Percent:** >98.0%(HPLC)(T)  
**CAS RN:** 83-67-0  
**Molecular Weight:** 180.17  
**Chemical Formula:** C<sub>7</sub>H<sub>8</sub>N<sub>4</sub>O<sub>2</sub>  
**Synonyms:** 3,7-Dimethylxanthine

**4. FIRST-AID MEASURES****Description of first aid measures**

<b>Inhalation:</b>	Remove victim to fresh air and keep at rest in a position comfortable for breathing. Get medical advice/attention if you feel unwell.
<b>Skin contact:</b>	Remove/Take off immediately all contaminated clothing. Rinse skin with water/shower. If skin irritation or rash occurs: Get medical advice/attention.
<b>Eye contact:</b>	Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. If eye irritation persists: Get medical advice/attention.
<b>Ingestion:</b>	Call a POISON CENTER or doctor/physician if you feel unwell. Rinse mouth.

**Symptoms/effects:**

<b>Acute:</b>	No data available
<b>Delayed:</b>	No data available

**Indication of any immediate medical attention:**

Not available.

**Notes to physician:**

No data available

**5. FIRE-FIGHTING MEASURES**

<b>Suitable extinguishing media:</b>	Dry chemical, foam, water spray, carbon dioxide.
<b>Specific hazards arising from the chemical:</b>	Take care as it may decompose upon combustion or in high temperatures to generate poisonous fume.
<b>Hazardous combustion products:</b>	These products include: Carbon oxides Nitrogen oxides
<b>Other specific hazards:</b>	Closed containers may explode from heat of a fire.
<b>Advice for firefighters:</b>	Wear self-contained breathing apparatus if possible.

**6. ACCIDENTAL RELEASE MEASURES**

<b>Personal precautions, protective equipment and emergency procedures:</b>	Use personal protective equipment. Keep people away from and upwind of spill/leak. Entry to non-involved personnel should be controlled around the leakage area by roping off, etc.
<b>Environmental precautions:</b>	Prevent product from entering drains.
<b>Methods and materials for containment and cleaning up:</b>	Sweep dust to collect it into an airtight container, taking care not to disperse it. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

**7. HANDLING AND STORAGE**

<b>Precautions for safe handling:</b>	Handling is performed in a well ventilated place. Wear suitable protective equipment. Prevent dispersion of dust. Wash hands and face thoroughly after handling. Use a local exhaust if dust or aerosol will be generated. Avoid contact with skin, eyes and clothing.
<b>Conditions for safe storage, including any incompatibilities</b>	
<b>Storage conditions:</b>	Keep container tightly closed. Store in a cool and dark place. Store away from incompatible materials such as oxidizing agents.
<b>Packaging material:</b>	Comply with laws.

**8. EXPOSURE CONTROLS / PERSONAL PROTECTION**

<b>Appropriate engineering controls:</b>	Follow safe industrial engineering/laboratory practices when handling any chemical. Install a closed system or local exhaust as possible so that workers should not be exposed directly. Also install safety shower and eye bath.
<b>Personal protective equipment</b>	
<b>Respiratory protection:</b>	Dust respirator. Follow local and national regulations.
<b>Hand protection:</b>	Protective gloves.
<b>Eye protection:</b>	Safety glasses. A face-shield, if the situation requires.
<b>Skin and body protection:</b>	Protective clothing. Protective boots, if the situation requires.

9. PHYSICAL AND CHEMICAL PROPERTIES
-------------------------------------

<b>Physical state (20°C):</b>	Solid		
<b>Form:</b>	Crystal - Powder		
<b>Colour:</b>	White - Slightly pale reddish yellow		
<b>Odour:</b>	No data available		
<b>Odor threshold:</b>	No data available		
<b>Odour threshold:</b>	No data available		
<b>Melting point/freezing point:</b>	350°C (662°F)	<b>pH:</b>	No data available
<b>Boiling point/range:</b>	No data available	<b>Vapour pressure:</b>	No data available.
<b>Decomposition temperature:</b>	No data available	<b>Vapour density:</b>	No data available
<b>Relative density:</b>	No data available	<b>Dynamic Viscosity:</b>	No data available
<b>Kinematic viscosity:</b>	No data available		
<b>Log Pow:</b>	No data available	<b>Evaporation rate(Butyl Acetate=1):</b>	No data available
<b>Flash point:</b>	No data available	<b>Autoignition temperature:</b>	No data available
<b>Flammability(solid, gas):</b>	No data available	<b>Flammability or explosive limits:</b>	
		<b>Lower:</b>	No data available
		<b>Upper:</b>	No data available
<b>Solubility(ies):</b>			
<b>[Water]</b>	No data available		
<b>[Other solvents]</b>			
<b>Soluble:</b>	Sodium hydroxide solution		

10. STABILITY AND REACTIVITY
------------------------------

<b>Reactivity:</b>	No data available
<b>Chemical stability:</b>	Stable under proper conditions.
<b>Possibility of hazardous reactions:</b>	No special reactivity has been reported.
<b>Incompatible materials:</b>	Oxidizing agents
<b>Hazardous decomposition products:</b>	Carbon dioxide, Carbon monoxide, Nitrogen oxides (NOx)

11. TOXICOLOGICAL INFORMATION
-------------------------------

RTECS Number: XH2275000

**Acute Toxicity:**  
 orl-rat LD50:1265 mg/kg scu-mus LD50:530 mg/kg

**Skin corrosion/irritation:**  
 No data available

**Serious eye damage/irritation:**  
 No data available

**Respiratory or skin sensitization:**  
 No data available

**Germ cell mutagenicity:**  
 dni-hmn-oth 4 mmol/L dns-hmn-oth 1 mmol/L  
 mmo-eug 600 mg/L (-S9)

**Carcinogenicity:**  
 No data available

**IARC:** Group 3 (Not classifiable as carcinogenic to humans).

**NTP:** No data available

**OSHA:** No data available

**Reproductive toxicity:**  
 ipr-mus TDLo: 500 mg/kg (13D preg) orl-mus TDLo: 6300 mg/kg (1-21D preg)

**Target organ(s):** No data available

**12. ECOLOGICAL INFORMATION****Ecotoxicity:**

<b>Fish:</b>	No data available
<b>Crustacea:</b>	No data available
<b>Algae:</b>	No data available

**Persistence / degradability:** No data available

**Bioaccumulative potential(BCF):** No data available

**Mobility in soil**

<b>Log Pow:</b>	No data available
<b>Soil adsorption (Koc):</b>	No data available
<b>Henry's Law (PaM<sup>3</sup>/mol):</b>	No data available

**13. DISPOSAL CONSIDERATIONS**

<b>Disposal of product:</b>	Recycle to process if possible. It is the generator's responsibility to comply with Federal, State and Local rules and regulations. 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. This section is intended to provide assistance but does not replace these laws, nor does compliance in accordance with this section ensure regulatory compliance according to the law. US EPA guidelines for Identification and Listing of Hazardous Waste are listed in 40 CFR Parts 261. The product should not be allowed to enter the environment, drains, water ways, or the soil.
<b>Disposal of container:</b>	Dispose of as unused product. Do not re-use empty containers.
<b>Other considerations:</b>	Observe all federal, state and local regulations when disposing of the substance.

**14. TRANSPORT INFORMATION**

<b>DOT (US)</b>	Non-hazardous for transportation.
<b>IATA</b>	Non-hazardous for transportation.
<b>IMDG</b>	Non-hazardous for transportation.

**15. REGULATORY INFORMATION****Toxic Substance Control Act (TSCA 8b.):**

This product is ON the EPA Toxic Substances Control Act (TSCA) inventory.

**US Federal Regulations****CERCLA Hazardous substance and Reportable Quantity:**

<b>SARA 313:</b>	Not Listed
<b>SARA 302:</b>	Not Listed

**State Regulations****State Right-to-Know**

<b>Massachusetts</b>	Not Listed
<b>New Jersey</b>	Not Listed
<b>Pennsylvania</b>	Not Listed
<b>California Proposition 65:</b>	Not Listed

**Other Information****NFPA Rating:**

<b>Health:</b>	1
<b>Flammability:</b>	0
<b>Instability:</b>	0

**HMIS Classification:**

<b>Health:</b>	1
<b>Flammability:</b>	0
<b>Physical:</b>	0

**International Inventories**

<b>Canada: NDSL</b>	On NDSL
<b>EC-No:</b>	201-494-2

**16. OTHER INFORMATION****Revision date:** 07/06/2018**Revision number:** 1

TCI chemicals are for research purposes only and are NOT intended for use as drugs, food additives, household, 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 affiliates or 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 SDS 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 SDS 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, face mask, fume hood). For proper handling and disposal, always comply with federal, state and local regulations.