



Health	2
Fire	1
Reactivity	0
Personal Protection	E

Material Safety Data Sheet

Theophylline MSDS

Section 1: Chemical Product and Company Identification

Product Name: Theophylline

Catalog Codes: SLT1348

CAS#: 58-55-9

RTECS: XH3850000

TSCA: TSCA 8(b) inventory: Theophylline

CI#: Not available.

Synonym: Acet-theocin; Armophylline; Asmax, Austyn, Duraphy, Elixicon, Elixophyllin, Elixophylline, Euphyllong, Lanophyllin, Liquophylline, Nuelin, Optiphyllin; Parkophyllin, Pseudotheophylline, Slo-Phyllin, Solosin, Teofyllamin, Theo-Dur, Teocin, Theofol, Theograd, Theolair, Theolix, Theophyllin; 1,3-Dimethyl-2,6-dihydroxypurine; 1,3-Dimethylxanthine; 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-

Chemical Name: Theophylline

Chemical Formula: C₇H₈N₄O₂

Contact Information:

Sciencelab.com, Inc.

14025 Smith Rd.

Houston, Texas 77396

US Sales: **1-800-901-7247**

International Sales: **1-281-441-4400**

Order Online: ScienceLab.com

CHEMTREC (24HR Emergency Telephone), call:
1-800-424-9300

International CHEMTREC, call: 1-703-527-3887

For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
Theophylline	58-55-9	100

Toxicological Data on Ingredients: Theophylline: ORAL (LD50): Acute: 225 mg/kg [Rat]. 235 mg/kg [Mouse]. 350 mg/kg [Rabbit].

Section 3: Hazards Identification

Potential Acute Health Effects:

Hazardous in case of ingestion. Slightly hazardous in case of skin contact (irritant), of eye contact (irritant), of inhalation.

Potential Chronic Health Effects:

CARCINOGENIC EFFECTS: Classified 3 (Equivocal evidence.) by NTP. 3 (Not classifiable for human.) by IARC.

MUTAGENIC EFFECTS: Mutagenic for mammalian somatic cells. Mutagenic for bacteria and/or yeast. **TERATOGENIC**

EFFECTS: Not available. **DEVELOPMENTAL TOXICITY:** Not available. The substance may be toxic to kidneys, the nervous system, heart, Smooth Muscle. Repeated or prolonged exposure to the substance can produce target organs damage.

Section 4: 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. Cold water may be used. Get medical attention if irritation occurs.

Skin Contact:

Wash with soap and water. Cover the irritated skin with an emollient. Get medical attention if irritation develops. Cold water may be used.

Serious Skin Contact: Not available.

Inhalation:

If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical attention.

Serious Inhalation: Not available.

Ingestion:

Do NOT induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. If large quantities of this material are swallowed, call a physician immediately. Loosen tight clothing such as a collar, tie, belt or waistband.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: May be combustible at high temperature.

Auto-Ignition Temperature: Not available.

Flash Points: Not available.

Flammable Limits: Not available.

Products of Combustion: These products are carbon oxides (CO, CO₂), nitrogen oxides (NO, NO₂...).

Fire Hazards in Presence of Various Substances:

Slightly flammable to flammable in presence of heat. Non-flammable in presence of shocks.

Explosion Hazards in Presence of Various Substances:

Slightly explosive in presence of open flames and sparks. Non-explosive in presence of shocks.

Fire Fighting Media and Instructions:

SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use water spray, fog or foam. Do not use water jet.

Special Remarks on Fire Hazards:

Material in powder form, capable of creating a dust explosion. As with most organic solids, fire is possible at elevated temperatures

Special Remarks on Explosion Hazards:

Fine dust dispersed in air in sufficient concentrations, and in the presences of an ignition source is a potential dust explosion hazard.

Section 6: Accidental Release Measures

Small Spill:

Use appropriate tools to put the spilled solid in a convenient waste disposal container. Finish cleaning by spreading water on the contaminated surface and dispose of according to local and regional authority requirements.

Large Spill:

Use a shovel to put the material into a convenient waste disposal container. Finish cleaning by spreading water on the contaminated surface and allow to evacuate through the sanitary system.

Section 7: Handling and Storage

Precautions:

Keep away from heat. Keep away from sources of ignition. Do not breathe dust. Wear suitable protective clothing. If ingested, seek medical advice immediately and show the container or the label.

Storage: Keep container tightly closed. Keep container in a cool, well-ventilated area.

Section 8: 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: Safety glasses. Lab coat. Dust respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

Personal Protection in Case of a Large Spill:

Splash goggles. Full suit. Dust respirator. Boots. Gloves. A self contained breathing apparatus should 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 9: Physical and Chemical Properties

Physical state and appearance: Solid. (Crystalline solid. Crystalline powder.)

Odor: Odorless.

Taste: Bitter.

Molecular Weight: 180.17 g/mole

Color: White.

pH (1% soln/water): Not available.

Boiling Point: Not available.

Melting Point: 274.5°C (526.1°F)

Critical Temperature: Not available.

Specific Gravity: Not available.

Vapor Pressure: Not applicable.

Vapor Density: Not available.

Volatility: Not available.

Odor Threshold: Not available.

Water/Oil Dist. Coeff.: The product is equally soluble in oil and water; $\log(\text{oil/water}) = -0.02$

Ionicity (in Water): Not available.

Dispersion Properties: See solubility in water.

Solubility:

Partially soluble in cold water. Very slightly soluble in diethyl ether. Soluble in dilute mineral acids. Water solubility: 7,400 mg/l @ 25 deg. C.

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Excess heat, dust generation

Incompatibility with various substances: Not available.

Corrosivity: Non-corrosive in presence of glass.

Special Remarks on Reactivity: Not available.

Special Remarks on Corrosivity: Not available.

Polymerization: Will not occur.

Section 11: Toxicological Information

Routes of Entry: Inhalation. Ingestion.

Toxicity to Animals: Acute oral toxicity (LD50): 225 mg/kg [Rat].

Chronic Effects on Humans:

CARCINOGENIC EFFECTS: Classified 3 (Equivocal evidence.) by NTP. 3 (Not classifiable for human.) by IARC.

MUTAGENIC EFFECTS: Mutagenic for mammalian somatic cells. Mutagenic for bacteria and/or yeast. May cause damage to the following organs: kidneys, the nervous system, heart, Smooth Muscle.

Other Toxic Effects on Humans:

Hazardous in case of ingestion. Slightly hazardous in case of skin contact (irritant), of inhalation.

Special Remarks on Toxicity to Animals:

Lowest Published Lethal Dose: LDL [Woman] - Route: Oral; Dose: 130 mg/kg

Special Remarks on Chronic Effects on Humans:

Human: passes through the placenta, excreted in maternal milk. May cause adverse reproductive effects and birth defects (teratogenic) May affect genetic material (mutagenic). May cause cancer based on animal test data.

Special Remarks on other Toxic Effects on Humans:

Acute Potential Health Effects: Skin: May cause skin irritation. Eyes: May cause eye irritation. Inhalation: May cause respiratory tract irritation. Ingestion: Harmful if swallowed. Can cause gastrointestinal tract irritation with nausea, vomiting, headache, vague abdominal discomfort, diarrhea, caffeine-like side effects insomnia, light-headedness, or a feeling of being "spaced-out." Other symptoms may include excitement, incoordination, tremor, hyperglycemia, metabolic acidosis, cardiac (ventricular)arrhythmias, hypotension, tachycardia, circulatory failure, respiratory stimulation, seizures/clonic and tonic convulsions, and death. Chronic Potential Health Effects: Ingestion: Prolonged or repeated ingestion may affect metabolism (weight loss), liver, urinary system (kidneys), blood (changes in white blood cell count, pigmented or nucleated red blood cells), brain, behavior/central nervous system (somnolence)

Section 12: Ecological Information

Ecotoxicity: Not available.

BOD5 and COD: Not available.

Products of Biodegradation:

Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

Toxicity of the Products of Biodegradation: The products of degradation are as toxic as the original product.

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:

Waste must be disposed of in accordance with federal, state and local environmental control regulations.

Section 14: Transport Information

DOT Classification: Not a DOT controlled material (United States).

Identification: Not applicable.

Special Provisions for Transport: Not applicable.

Section 15: Other Regulatory Information

Federal and State Regulations: TSCA 8(b) inventory: Theophylline

Other Regulations:

OSHA: Hazardous by definition of Hazard Communication Standard (29 CFR 1910.1200). EINECS: This product is on the European Inventory of Existing Commercial Chemical Substances.

Other Classifications:

WHMIS (Canada): CLASS D-1B: Material causing immediate and serious toxic effects (TOXIC).

DSCL (EEC):

R22- Harmful if swallowed. S36- Wear suitable protective clothing.

HMIS (U.S.A.):

Health Hazard: 2

Fire Hazard: 1

Reactivity: 0

Personal Protection: E

National Fire Protection Association (U.S.A.):

Health: 2

Flammability: 1

Reactivity: 0

Specific hazard:

Protective Equipment:

Gloves. Lab coat. Dust respirator. Be sure to use an approved/certified respirator or equivalent. Wear appropriate respirator when ventilation is inadequate. Safety glasses.

Section 16: Other Information

References: Not available.

Other Special Considerations: Not available.

Created: 10/10/2005 12:03 AM

Last Updated: 11/01/2010 12:00 PM

The information above is believed to be accurate and represents the best information currently available to us. However, we make no warranty of merchantability or any other warranty, express or implied, with respect to such information, and we assume

no liability resulting from its use. Users should make their own investigations to determine the suitability of the information for their particular purposes. In no event shall ScienceLab.com be liable for any claims, losses, or damages of any third party or for lost profits or any special, indirect, incidental, consequential or exemplary damages, howsoever arising, even if ScienceLab.com has been advised of the possibility of such damages.