MATERIAL SAFETY DATA SHEET

NAME OF PRODUCT: Theophylline MSDS DATE: 10 Jun, 2011

Notice

NSF Reference Standards are for test and assay use only and are not intended for human or animal consumption. This document communicates information relating to test and assay use only and may not be applicable for any unauthorized use.

SECTION 1: PRODUCT AND COMPANY IDENTIFICATION

Product Name:	Theophylline
Catalog Code:	RS1-0034
Synonym:	Acet-theocin; 1,3-Dimethyl-2,6-dihydroxypurine; 1,3 Dimethylxanthine; 1,3-dimethyl-7H-purine-2,6-dione
Chemical Formula:	$C_7H_8N_4O_2$
CAS #:	58-55-9

Contact Information:

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SECTION 2: COMPOSITION/INFORMATION ON INGREDIENTS

Name: Theophylline

CAS#: 58-55-9

% by Weight: 100%

Toxicological Data on Ingredients:
ORAL LD50: 235 mg/kg (Mouse): 225 mg/ kg (Rat): 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/ yeasts.
TERATOGENIC EFFECTS: Not available
DEVELOPMENTAL TOXICITY: Not available

Theophylline is toxic to kidneys, the nervous system, heart, and smooth muscle. Repeated or prolonged exposure to Theophylline can produce target organ damage.

SECTION 4: FIRST AID MEASURES

Eye Contact:
Check for and remove contact lenses. In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. Seek medical attention.
Skin Contact:
In case of contact, immediately wash skin with non-abrasive soap and plenty of water. Cover the irritated skin with an emollient. Seek medical attention if irritation persists.
Serious Skin Contact:
Not available.
Inhalation:
If inhaled, remove to fresh air. If large quantities of this material are swallowed, seek immediate medical attention.
Serious Inhalation:
Not available
Ingestion:
Do not induce vomiting. Loosen tight clothing. If victim is not breathing, perform mouth to mouth resuscitation. Seek immediate medical attention.
Serious Ingestion: Not available.

SECTION 5: FIRE-FIGHTING MEASURES

Flammability of the Product: May be combustible at high temperature.
Auto-Ignition Temperature: Not available.
Flammable Limits: Not available.

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Flash Points: Not available
Products of Combustion: These products are carbon oxides (CO, CO2), nitrogen oxides (NO, NO2…).
Special Remarks on Explosion Hazards: Not available.

Fire Hazards in Presence of Various Substances:
Slightly flammable to flammable in presence of heat. Non flammable in presence of shock.
Explosion Hazards in Presence of Various Substances:
Risks of explosion of the product in presence of mechanical impact: Not available.
Risks of explosion of the product in presence of static discharge: Not available.
Special Remarks on Fire Hazards: Material in powder form is capable of creating a dust explosion. As with most organic solids, fire is possible at high temperatures.

Fire Fighting Media and Instructions:
SMALL FIRE: Use DRY chemical powder.
LARGE FIRE: Use water spray, fog or foam. Do not use water jet.

SECTION 6: ACCIDENTAL RELEASE MEASURES

Small Spill:
Use appropriate tools to put the spilled solid in a convenient waste disposal container. After powder clean up, spread water on the contaminated surface and dispose of according to local and regional authority requirements.

Large Spill:
Use appropriate tools to put the material into a suitable waste disposal container. After powder clean up, spread water on the contaminated surface and dispose of according to local and regional authority requirements.

SECTION 7: HANDLING AND STORAGE

Precautions:
Keep away from heat. Keep away from sources of ignition. Ground all equipment containing material. Do not ingest. Do not breathe dust. Wear suitable protective clothing. In case of insufficient ventilation, wear suitable respiratory equipment. If ingested, seek medical advice immediately and show the container or the label. Avoid contact with skin and eyes.

Storage:
Keep container tightly closed. Keep container in a cool, well-ventilated area. Combustible materials should be stored away from extreme heat and away from strong oxidizing agents.

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SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

Engineering Controls:
If laboratory operations generate dust, use local exhaust ventilation or other appropriate engineering controls to keep exposure to airborne contaminants below the exposure limit.
Personal Protection:
Splash goggles. 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/ 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.: Theophylline is equally soluble in oil and water.
Ionicity (in Water): Not available.
Dispersion Properties: Not Available
Solubility: Partially soluble in cold water. Very slightly soluble in diethyl ether. Soluble in dilute mineral acids. Water solubility 7,400 mg/L @ 25 degrees C.

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SECTION 10: STABILITY AND REACTIVITY

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/ yeasts. Theophylline is toxic to kidneys, the nervous system, heart, and 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 located published Lethal dose LDL [woman] Oral 130 mg/kg

Special Remarks on Chronic Effects on Humans:
Not available.

Special Remarks on other Toxic Effects on Humans:
Acute potential health effects:

Skin: May cause irritation
Eyes: May cause irritation
Inhalation: May cause respiratory tract irritation.
Ingestion: Harmful if swallowed, can cause GI tract irritation

Prolonged or repeated ingestion may affect metabolism, liver, urinary system (kidneys), blood, brain, behavior/ CNS.

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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 product itself.
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 in the United States
Identification: Not applicable.
Special Provisions for Transport: Not applicable.

SECTION 15: 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: Theophylline is on the European inventory of existing commercial substances.

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

DSCL (EEC):
R22 – Harmful if swallowed. R36 – Wear suitable protective clothing.

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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. Safety glasses.

SECTION 16: OTHER INFORMATION

References: Not available.
Other Special Considerations: Not available.

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