1. Identification

Product identifier: Theophylline Melting Point Standard

Other means of identification:
- Catalog number: 1653117
- CAS number: 58-55-9
- Chemical name: 1-H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-

Recommended use:
Specified quality tests and assay use only.

Recommended restrictions:
Not for use as a drug. Not for administration to humans or animals.

Manufacturer/Importer/Supplier/Distributor information

Manufacturer:
- Company name: U. S. Pharmacopeia
- Address: 12601 Twinbrook Parkway, Rockville, MD, 20852-1790, United States
- Telephone: RS Technical Services 301-816-8129
- Website: www.usp.org
- E-mail: RSTECH@usp.org
- Emergency phone number:
  - CHEMTREC within US & Canada: 1-800-424-9300
  - CHEMTREC outside US & Canada: +1 703-527-3887

2. Hazard(s) identification

Physical hazards:
Not classified.

Health hazards:
- Acute toxicity, oral Category 3

Environmental hazards:
Not classified.

OSHA defined hazards:
Not classified.

Label elements

Signal word: Danger
Hazard statement: Toxic if swallowed.

Precautionary statement:
- Prevention: Wash thoroughly after handling.
- Storage:
- Disposal: Dispose of contents/container in accordance with local/regional/national/international regulations.

Hazard(s) not otherwise classified (HNOC):
None known.

Supplemental information:
Pharmacologically active material.

3. Composition/information on ingredients

Substance
<table>
<thead>
<tr>
<th>Chemical name</th>
<th>Common name and synonyms</th>
<th>CAS number</th>
<th>%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Theophylline Melting Point Standard</td>
<td></td>
<td>58-55-9</td>
<td>100</td>
</tr>
</tbody>
</table>

### 4. First-aid measures

#### Inhalation
Move to fresh air. Call a physician if symptoms develop or persist.

#### Skin contact
Rinse skin with water/shower. Get medical attention if irritation develops and persists.

#### Eye contact
Rinse with water. Get medical attention if irritation develops and persists.

#### Ingestion
IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician. Rinse mouth. Do not induce vomiting without advice from poison control center. If vomiting occurs, keep head low so that stomach content doesn’t get into the lungs.

**Most important symptoms/effects, acute and delayed**
Pharmacologically active material. Occupational exposure may cause physiological effects.

**Indication of immediate medical attention and special treatment needed**
Provide general supportive measures and treat symptomatically. Treatment of overdose may include the following: DO NOT induce vomiting. Administer activated charcoal as a slurry. Perform gastric lavage soon after ingestion (within one hour). Protect airway by placement in the Trendelenburg and left lateral decubitus position or by endotracheal intubation. In severely poisoned patients, consider multi-dose activated charcoal. Carthartics are NOT recommended. Persistent vomiting may interfere with activated charcoal administration. Treat with ranitidine, ondansetron, or metoclopramide. In patients with high risk for seizures, perform seizure prophylaxis with phenobarbital. For seizures, administer intravenous diazepam or lorazepam. Monitor for hypotension, respiratory depression, and need for endotracheal intubation. For hypotension, administer saline and place in Trendelenburg position. For severe tachycardia with hemodynamic compromise or ischemia, treat with beta blocking agents until hemodialysis or hemoperfusion can be performed. A short-acting cardioselective agent, such as esmolol, is preferred. Use CAUTION in patients with asthma or COPD. Begin intravenous hydration and replace electrolytes as needed. Obtain serial theophylline levels, follow serum electrolytes, Obtain an ECG, and institute continuous cardiac monitoring. For life threatening toxicity (significant dysrhythmias, hypotension, seizures), treat with hemoperfusion or hemodialysis.

### General information
Remove from exposure. Remove contaminated clothing. For treatment advice, seek guidance from an occupational health physician or other licensed health-care provider familiar with workplace chemical exposures. In the United States, the national poison control center phone number is 1-800-222-1222. If person is not breathing, give artificial respiration. If breathing is difficult, give oxygen if available. Persons developing serious hypersensitivity (anaphylactic) reactions must receive immediate medical attention.

### 5. Fire-fighting measures

#### Suitable extinguishing media
Water. Foam. Dry chemical or CO2. Use fire-extinguishing media appropriate for surrounding materials.

#### Unsuitable extinguishing media
None known.

#### Specific hazards arising from the chemical
No unusual fire or explosion hazards noted.

#### Special protective equipment and precautions for firefighters
Wear suitable protective equipment.

#### Fire fighting equipment/instructions
Use water spray to cool unopened containers. As with all fires, evacuate personnel to a safe area. Firefighters should use self-contained breathing equipment and protective clothing.

#### Specific methods
Use standard firefighting procedures and consider the hazards of other involved materials.

#### General fire hazards
No unusual fire or explosion hazards noted.

### 6. Accidental release measures

#### Personal precautions, protective equipment and emergency procedures
Keep unnecessary personnel away. Wear appropriate personal protective equipment. Avoid inhalation of dust from the spilled material. Do not touch damaged containers or spilled material unless wearing appropriate protective clothing. Ensure adequate ventilation. For personal protection, see section 8 of the SDS.

#### Methods and materials for containment and cleaning up
For waste disposal, see section 13 of the SDS. Avoid the generation of dusts during clean-up. Sweep up or vacuum up spillage and collect in suitable container for disposal. Clean surface thoroughly to remove residual contamination.

#### Environmental precautions
Avoid discharge into drains, water courses or onto the ground.
7. Handling and storage

Precautions for safe handling
As a general rule, when handling USP Reference Standards, avoid all contact and inhalation of dust, mists, and/or vapors associated with the material. Clean equipment and work surfaces with suitable detergent or solvent after use. After removing gloves, wash hands and other exposed skin thoroughly. Select and use containment devices and personal protective equipment based on a risk assessment of material potency and exposure potential.

Conditions for safe storage, including any incompatibilities
Store in tight container as defined in the USP-NF. This material should be handled and stored per label instructions to ensure product integrity.

8. Exposure controls/personal protection

Occupational exposure limits
No exposure limits noted for ingredient(s).

Biological limit values
No biological exposure limits noted for the ingredient(s).

Appropriate engineering controls
For laboratory operations, use local exhaust ventilation or a ventilated enclosure for high energy operations such as particle sizing. Control exposures to below the occupational exposure level (if available). Select and use containment devices and personal protective equipment based on a risk assessment of exposure potential. Cover all containers for solutions and slurries while being transferred.

Individual protection measures, such as personal protective equipment

Eye/face protection
Wear safety glasses with side shields, chemical splash goggles, or full face shield, if necessary. Base the choice of protection on the job activity and potential for contact with eyes or face. An emergency eye wash station should be available.

Skin protection

Hand protection
Wear nitrile or other impervious gloves if skin contact is possible. When the material is dissolved or suspended in an organic solvent, wear gloves that provide protection against the solvent.

Other
Train employees in proper gowning and degowning practices. Wear lab coat. Base the choice of skin protection on the job activity, potential for skin contact and solvents and reagents in use. Do not wear protective garments in common areas (e.g., cafeterias) or out-of-doors.

Respiratory protection
Respirators are generally not required for laboratory operations. Use a tight-fitting full-face respirator with HEPA filters for spill cleanup. Choose respiratory protection appropriate to the task and the level of existing engineering controls.

Thermal hazards
Wear appropriate thermal protective clothing, when necessary.

9. Physical and chemical properties

Appearance descriptions are general information and not specific to any USP lot.

Physical state
Solid.

Form
Crystalline powder.

Color
White.

Odor
Odorless.

Odor threshold
Not available.

pH
Not available.

Melting point/freezing point
518.54 - 525.56 °F (270.3 - 274.2 °C)

Initial boiling point and boiling range
Not available.

Flash point
Not available.

Evaporation rate
Not available.

Flammability (solid, gas)
Not available.

Upper/lower flammability or explosive limits

Flammability limit - lower (%)
Not available.

Flammability limit - upper (%)
Not available.

Explosive limit - lower (%)
Not available.

Explosive limit - upper (%)
Not available.

Vapor pressure
< 0.0000001 kPa at 25 °C
Vapor density Not available.
Relative density Not available.
Solubility(ies)
   Solubility (water) Slightly soluble.
   Solubility (other) Alcohol: Sparingly soluble.
                     Ammonia: Freely soluble.
                     Chloroform: Sparingly soluble.
                     Ether: Sparingly soluble.
Partition coefficient (n-octanol/water) -0.02
Auto-ignition temperature Not available.
Decomposition temperature Not available.
Viscosity Not available.
Other information
   Chemical family Xanthine.
   Molecular formula C7-H8-N4-O2
   Molecular weight 180.17 g/mol
   pH in aqueous solution 4 - 6 Solution: 2%
10. Stability and reactivity
Reactivity The product is stable and non-reactive under normal conditions of use, storage and transport.
Chemical stability Material is stable under normal conditions.
Possibility of hazardous reactions No dangerous reaction known under conditions of normal use.
Conditions to avoid Contact with incompatible materials.
Incompatible materials Alkaline metals. Peroxides.
Hazardous decomposition products Irritating and/or toxic fumes or gases. Emits toxic fumes under fire conditions. NOx.
11. Toxicological information
Information on likely routes of exposure
   Inhalation Knowledge about health hazard is incomplete.
   Skin contact Knowledge about health hazard is incomplete.
   Eye contact Knowledge about health hazard is incomplete.
   Ingestion Toxic if swallowed.
Information on toxicological effects
   Acute toxicity Toxic if swallowed.
   Test Results

<table>
<thead>
<tr>
<th>Product</th>
<th>Species</th>
<th>Test Results</th>
</tr>
</thead>
<tbody>
<tr>
<td>Theophylline Melting Point Standard (CAS 58-55-9)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Acute Oral</td>
<td>Rat</td>
<td>225 mg/kg</td>
</tr>
<tr>
<td>LD50</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Skin corrosion/irritation Based on available data, the classification criteria are not met.
Serious eye damage/eye irritation Based on available data, the classification criteria are not met.
Local effects
   Eye irritation, undiluted
   Result: Not irritating.
   Species: Rabbit
Local effects
Skin irritation, 50% aqueous dilution
Result: Not irritating.
Species: Rabbit

Respiratory or skin sensitization
Respiratory sensitization
Knowledge about health hazard is incomplete.
Skin sensitization
Knowledge about health hazard is incomplete.

Germ cell mutagenicity
Knowledge about mutagenicity is incomplete.

Mutagenicity
Ames test (Salmonella typhimurium)
Result: Negative.
Micronucleus assay
Result: Negative.
Mutagenicity: Chinese hamster ovary assay
Result: Negative.
Mutagenicity: In vivo cytopigenic study
Result: Negative.

Carcinogenicity
Based on available data, the classification criteria are not met.

75 - 150 mg/kg Carcinogenicity
Result: No evidence of carcinogenicity.
Species: Mouse
Test Duration: 2 years
75 mg/kg Carcinogenicity
Result: No evidence of carcinogenicity.
Species: Rat
Test Duration: 2 years

IARC Monographs, Overall Evaluation of Carcinogenicity
Theophylline Melting Point Standard (CAS 58-55-9) 3 Not classifiable as to carcinogenicity to humans.

OSHA Specifically Regulated Substances (29 CFR 1910.1001-1050)
Not regulated.

US. National Toxicology Program (NTP) Report on Carcinogens
Not listed.

Reproductive toxicity
Based on available data, the classification criteria are not met.
Several large studies of infants born to women treated with theophylline during pregnancy showed no increase in birth defects.

Reproductivity
15 mg/kg/day Reproductive
Result: Dose-related increase in birth defects (cleft palate, skeletal anomalies) in offspring.
Species: Rabbit
259 mg/kg/day Reproductive
Result: No significant increase in birth defects.
Species: Rat
396 mg/kg/day Reproductive
Result: No significant increase in birth defects.
Species: Mouse
Reproductive, (6 to 25 times the human dose)
Result: Dose-related increase in birth defects (cleft palate, skeletal anomalies) observed in offspring treated at high doses.
Species: Rat

Specific target organ toxicity - single exposure
Knowledge about health hazard is incomplete.

Specific target organ toxicity - repeated exposure
Knowledge about health hazard is incomplete.

Aspiration hazard
Based on available data, the classification criteria are not met.

Further information
Pharmacologically active material. Occupational exposure may cause physiological effects.

12. Ecological information
Ecotoxicity
The product is not classified as environmentally hazardous. However, this does not exclude the possibility that large or frequent spills can have a harmful or damaging effect on the environment.

Persistence and degradability
No data is available on the degradability of this product.
Bioaccumulative potential

Octanol/water partition coefficient log Kow

-0.02

Mobility in soil

No data available.

Other adverse effects

No other adverse environmental effects (e.g. ozone depletion, photochemical ozone creation potential, endocrine disruption, global warming potential) are expected from this component.

13. Disposal considerations

Disposal instructions

Dispose in accordance with all applicable regulations. Under RCRA, it is the responsibility of the user of the product to determine, at the time of disposal, whether the product meets RCRA criteria for hazardous waste.

Local disposal regulations

Dispose in accordance with all applicable regulations.

Hazardous waste code

The waste code should be assigned in discussion between the user, the producer and the waste disposal company.

Waste from residues / unused products

Empty containers or liners may retain some product residues. This material and its container must be disposed of in a safe manner (see: Disposal instructions).

Contaminated packaging

Since emptied containers may retain product residue, follow label warnings even after container is emptied.

14. Transport information

DOT

UN number: UN2811

UN proper shipping name: Toxic solid, organic, n.o.s. (Theophylline)

Class: 6.1

Subsidiary risk: -

Packing group: III

Packaging exceptions: 153

Packaging non bulk: 213

Packaging bulk: 240

IATA

UN number: UN2811

UN proper shipping name: Toxic solid, organic, n.o.s. (Theophylline)

Class: 6.1

Subsidiary risk: -

Packing group: III

Other information

Passenger and cargo aircraft: Allowed with restrictions.

Cargo aircraft only: Allowed with restrictions.

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

DOT; IATA

General information

It is the shipper's responsibility to determine the correct transport classification at the time of shipment.
15. Regulatory information

**US federal regulations**

CERCLA/SARA Hazardous Substances - Not applicable.

All components are on the U.S. EPA TSCA Inventory List. This product is a "Hazardous Chemical" as defined by the OSHA Hazard Communication Standard, 29 CFR 1910.1200.

**TSCA Section 12(b) Export Notification (40 CFR 707, Subpt. D)**

Not regulated.

**CERCLA Hazardous Substance List (40 CFR 302.4)**

Not listed.

**SARA 304 Emergency release notification**

Not regulated.


Not regulated.

**Superfund Amendments and Reauthorization Act of 1986 (SARA)**

<table>
<thead>
<tr>
<th>Hazard categories</th>
<th>Immediate Hazard - Yes</th>
<th>Delayed Hazard - No</th>
<th>Fire Hazard - No</th>
<th>Pressure Hazard - No</th>
<th>Reactivity Hazard - No</th>
</tr>
</thead>
</table>

**SARA 302 Extremely hazardous substance**

Not listed.

**SARA 311/312 Hazardous chemical**

Yes

**SARA 313 (TRI reporting)**

Not regulated.

**Other federal regulations**

**Clean Air Act (CAA) Section 112 Hazardous Air Pollutants (HAPs) List**

Not regulated.

**Clean Air Act (CAA) Section 112(r) Accidental Release Prevention (40 CFR 68.130)**

Not regulated.

**Safe Drinking Water Act (SDWA)**

Not regulated.

**US state regulations**

California Safe Drinking Water and Toxic Enforcement Act of 1986 (Proposition 65): This material is not known to contain any chemicals currently listed as carcinogens or reproductive toxins.

**International Inventories**

<table>
<thead>
<tr>
<th>Country(s) or region</th>
<th>Inventory name</th>
<th>On inventory (yes/no)*</th>
</tr>
</thead>
<tbody>
<tr>
<td>Australia</td>
<td>Australian Inventory of Chemical Substances (AICS)</td>
<td>Yes</td>
</tr>
<tr>
<td>Canada</td>
<td>Domestic Substances List (DSL)</td>
<td>Yes</td>
</tr>
<tr>
<td>Canada</td>
<td>Non-Domestic Substances List (NDSL)</td>
<td>No</td>
</tr>
<tr>
<td>China</td>
<td>Inventory of Existing Chemical Substances in China (IECSC)</td>
<td>Yes</td>
</tr>
<tr>
<td>Europe</td>
<td>European Inventory of Existing Commercial Chemical Substances (EINECS)</td>
<td>Yes</td>
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<tr>
<td>Europe</td>
<td>European List of Notified Chemical Substances (ELINCS)</td>
<td>No</td>
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<tr>
<td>Japan</td>
<td>Inventory of Existing and New Chemical Substances (ENCS)</td>
<td>Yes</td>
</tr>
<tr>
<td>Korea</td>
<td>Existing Chemicals List (ECL)</td>
<td>Yes</td>
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<tr>
<td>New Zealand</td>
<td>New Zealand Inventory</td>
<td>Yes</td>
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<tr>
<td>Philippines</td>
<td>Philippine Inventory of Chemicals and Chemical Substances (PICCS)</td>
<td>Yes</td>
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<tr>
<td>United States &amp; Puerto Rico</td>
<td>Toxic Substances Control Act (TSCA) Inventory</td>
<td>Yes</td>
</tr>
</tbody>
</table>

*A "Yes" indicates that all components of this product comply with the inventory requirements administered by the governing country(s).

A "No" indicates that one or more components of the product are not listed or exempt from listing on the inventory administered by the governing country(s).

16. Other information, including date of preparation or last revision

**Issue date**

01-29-2007
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