



# SAFETY DATA SHEET

## 1. Identification

|   |   |                 |
|---|---|-----------------|
| <b>Product identifier</b>                                     | <b>Caffeine Melting Point Standard</b>                                    |                 |
| <b>Other means of identification</b>                          |   |                 |
| <b>Catalog number</b>   | 1086006   |                 |
| <b>CAS number</b>   | 58-08-2   |                 |
| <b>Synonyms</b>   | 1,3,7-Trimethylxanthine   |                 |
| <b>Chemical name</b>  | 1H-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl-                         |                 |
| <b>Recommended use</b>  | Specified quality tests and assay use only.                               |                 |
| <b>Recommended restrictions</b>                               | Not for use as a drug. Not for administration to humans or animals.       |                 |
| <b>Manufacturer/Importer/Supplier/Distributor information</b> |   |                 |
| <b>Manufacturer</b>   |   |                 |
| <b>Company name</b>   | U. S. Pharmacopeia  |                 |
| <b>Address</b>  | 12601 Twinbrook Parkway<br>Rockville<br>MD<br>20852-1790<br>United States |                 |
| <b>Telephone</b>  | RS Technical Services   | 301-816-8129    |
| <b>Website</b>  | www.usp.org   |                 |
| <b>E-mail</b>   | RSTECH@usp.org  |                 |
| <b>Emergency phone number</b>                                 | CHEMTREC within US & Canada   | 1-800-424-9300  |
|   | CHEMTREC outside US & Canada  | +1 703-527-3887 |

## 2. Hazard(s) identification

|                              |                            |            |
|------------------------------|----------------------------|------------|
| <b>Physical hazards</b>      | Not classified.            |            |
| <b>Health hazards</b>        | Acute toxicity, oral       | Category 3 |
|                              | Acute toxicity, inhalation | Category 4 |
| <b>Environmental hazards</b> | Not classified.            |            |
| <b>OSHA defined hazards</b>  | Not classified.            |            |
| <b>Label elements</b>        |                            |            |



|  |  |  |
|--|--|--|
| <b>Signal word</b>                               | Danger   |  |
| <b>Hazard statement</b>                          | Toxic if swallowed. Harmful if inhaled.  |  |
| <b>Precautionary statement</b>                   |  |  |
| <b>Prevention</b>                                | Avoid breathing dust/fume. Wash thoroughly after handling. Use only outdoors or in a well-ventilated area.   |  |
| <b>Response</b>                                  | If swallowed: Immediately call a poison center/doctor. Rinse mouth. If inhaled: Remove person to fresh air and keep comfortable for breathing. Call a poison center/doctor if you feel unwell. |  |
| <b>Storage</b>                                   | Store locked up.   |  |
| <b>Disposal</b>                                  | Dispose of contents/container in accordance with local/regional/national/international regulations.  |  |
| <b>Hazard(s) not otherwise classified (HNOC)</b> | None known.  |  |
| <b>Supplemental information</b>                  | Pharmacologically active material.   |  |

### 3. Composition/information on ingredients

#### Substance

| Chemical name                   | Common name and synonyms | CAS number | %   |
|---------------------------------|--------------------------|------------|-----|
| Caffeine Melting Point Standard | 1,3,7-Trimethylxanthine  | 58-08-2    | 100 |

### 4. First-aid measures

|   |  |
|---|--|
| <b>Inhalation</b>   | If breathing is difficult, remove to fresh air and keep at rest in a position comfortable for breathing. Do not use mouth-to-mouth method if the substance is inhaled. Call a physician if symptoms develop or persist.  |
| <b>Skin contact</b>   | Rinse skin with water/shower. Get medical attention if irritation develops and persists.   |
| <b>Eye contact</b>  | Rinse with water. Get medical attention if irritation develops and persists.   |
| <b>Ingestion</b>  | Rinse mouth. If vomiting occurs, keep head low so that stomach content doesn't get into the lungs. Do not induce vomiting without advice from poison control center. Call a physician or poison control center immediately.  |
| <b>Most important symptoms/effects, acute and delayed</b>                     | Cardiovascular effects. Central nervous system effects. Pharmacologically active material. Occupational exposure may cause physiological effects.  |
| <b>Indication of immediate medical attention and special treatment needed</b> | Provide general supportive measures and treat symptomatically. Treatment of overdose may include the following: Do NOT induce vomiting. Administer activated charcoal as a slurry. For seizures, administer intravenous diazepam or lorazepam. If seizures recur, consider phenobarbital. For gastrointestinal irritation in stable patients, administer liquid antacids, as needed. Monitor fluid and electrolyte status and correct abnormalities. Hyperkalemia is common. For rhabdomyolysis, ensure adequate hydration and urine output. Treat life-threatening dysrhythmias and those that compromise hemodynamic status aggressively. Dysrhythmias often respond to beta-blockers. For ventricular dysrhythmias, institute continuous cardiac monitoring, obtain an ECG, and administer oxygen. Evaluate for hypoxia, acidosis and electrolyte disorders. Lidocaine and amiodarone are first line agents for stable monomorphic ventricular tachycardia, particularly in patients with underlying impaired cardiac function. Sotalol is an alternative. Use amiodarone and sotalol with caution with prolongation of QT interval and/or torsades de pointes. Unstable rhythms require cardioversion. For severe tachycardia in hemodynamically unstable patients, treat with short acting cardioselective beta-blocker, like esmolol. Propranolol is an alternative. For hypotension, infuse isotonic fluid. If hypotension persists, administer dopamine or norepinephrine. Hemoperfusion is more effective than dialysis in enhancing elimination. |
| <b>General information</b>  | 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

|  |   |
|--|---|
| <b>Suitable extinguishing media</b>                                  | Water. Foam. Dry chemical or CO <sub>2</sub> . Use fire-extinguishing media appropriate for surrounding materials.                        |
| <b>Unsuitable extinguishing media</b>                                | None known.   |
| <b>Specific hazards arising from the chemical</b>                    | No unusual fire or explosion hazards noted.   |
| <b>Special protective equipment and precautions for firefighters</b> | Wear suitable protective equipment.   |
| <b>Fire fighting equipment/instructions</b>                          | As with all fires, evacuate personnel to a safe area. Firefighters should use self-contained breathing equipment and protective clothing. |
| <b>Specific methods</b>  | Cool containers exposed to flames with water until well after the fire is out.  |
| <b>General fire hazards</b>  | No unusual fire or explosion hazards noted.   |

### 6. Accidental release measures

|  |  |
|--|--|
| <b>Personal precautions, protective equipment and emergency procedures</b> | 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. |
| <b>Methods and materials for containment and cleaning up</b>               | 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

The following constituents are the only constituents of the product which have a PEL, TLV or other recommended exposure limit. At this time, the other constituents have no known exposure limits.

### Exposure limit values

#### Industrial Use Material

#### Type

#### Value

| Industrial Use Material                       | Type | Value             |
|---|------|-------------------|
| Caffeine Melting Point Standard (CAS 58-08-2) | TWA  | 200 micrograms/m3 |

### 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.

### General hygiene considerations

Handling practices in this SDS are recommendations for laboratory use of reference standards. Procedures for any other uses or quantities should be determined after an appropriate assessment.

## 9. Physical and chemical properties

### Appearance

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

#### Physical state

Solid.

#### Form

Powder. Needles.

#### Color

White.

### Odor

Odorless.

### Odor threshold

Not available.

### pH

Not available.

### Melting point/freezing point

455 - 462.2 °F (235 - 239 °C)

### Initial boiling point and boiling range

352.4 °F (178 °C) (sublimes)

### Flash point

Not available.

### Evaporation rate

Not available.

### Flammability (solid, gas)

Not available.

**Upper/lower flammability or explosive limits**

|                                       |                |
|---------------------------------------|----------------|
| <b>Flammability limit - lower (%)</b> | Not available. |
| <b>Flammability limit - upper (%)</b> | Not available. |
| <b>Explosive limit - lower (%)</b>    | Not available. |
| <b>Explosive limit - upper (%)</b>    | Not available. |

**Vapor pressure** 15 mm Hg at 89 °C

**Vapor density** Not available.

**Relative density** Not available.

**Solubility(ies)**

|                           |  |
|---------------------------|--|
| <b>Solubility (water)</b> | Sparingly soluble.   |
| <b>Solubility (other)</b> | Ethanol: sparingly soluble<br>Ether: slightly soluble<br>Pyrrole: freely soluble<br>Chloroform: freely soluble<br>Ethyl acetate: soluble |

**Partition coefficient (n-octanol/water)** -0.091 = Log Pow at 23 °C

**Auto-ignition temperature** > 1112 °F (> 600 °C) (DIN 51794)  
1697 °F (925 °C)

**Decomposition temperature** Not available.

**Viscosity** Not available.

**Other information**

|                               |  |
|-------------------------------|--|
| <b>Chemical family</b>        | Methylated xanthine.   |
| <b>Molecular formula</b>      | C <sub>8</sub> H <sub>10</sub> N <sub>4</sub> O <sub>2</sub> |
| <b>Molecular weight</b>       | 194.19   |
| <b>Percent volatile</b>       | 0 %  |
| <b>pH in aqueous solution</b> | 5.5 - 6.9  |
| <b>Specific gravity</b>       | 1.23 at 18 °C  |

**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** Strong oxidizing agents. Alkaline metals. Phenols. Tannins. Caustic solutions.

**Hazardous decomposition products** NO<sub>x</sub>. Irritating and/or toxic fumes or gases. Emits toxic fumes under fire conditions.

**11. Toxicological information****Information on likely routes of exposure**

|                     |  |
|---------------------|--|
| <b>Inhalation</b>   | Harmful if inhaled.  |
| <b>Skin contact</b> | Knowledge about health hazard is incomplete.   |
| <b>Eye contact</b>  | Knowledge about health hazard is incomplete.   |
| <b>Ingestion</b>    | Toxic if swallowed. This material may cause: Central nervous system effects. Cardiovascular effects. |

**Symptoms related to the physical, chemical and toxicological characteristics** Xanthine derivatives: Gastrointestinal disturbances. Fast or irregular heartbeat. Flushing. Dizziness. Trembling. Convulsions. Shortness of breath. Headache. Increased urination. Mood or mental changes.

**Information on toxicological effects**

**Acute toxicity** Toxic if swallowed. Harmful if inhaled.

| Product   | Species   | Test Results  |
|---|---|---|
| Caffeine Melting Point Standard (CAS 58-08-2)                         |   |   |
| <b>Oral</b>   |   |   |
| LD50  | Rat   | 192 mg/kg   |
| <b>Acute</b>  |   |   |
| <b>Dermal</b>   |   |   |
| LD50  | Rat   | > 2000 mg/kg  |
| <b>Inhalation</b>   |   |   |
| LC50  | Rat   | 4.94 mg/l, 4 hours                                  |
| <b>Skin corrosion/irritation</b>                                      | Based on available data, the classification criteria are not met.   |   |
| <b>Serious eye damage/eye irritation</b>                              | Based on available data, the classification criteria are not met.   |   |
| <b>Local effects</b>  |   |   |
| Irritancy - OECD 404  |   |   |
| Result: Not irritant.   |   |   |
| Species: Rabbit   |   |   |
| Organ: Skin   |   |   |
| Irritancy - OECD 405  |   |   |
| Result: Not irritant.   |   |   |
| Species: Rabbit   |   |   |
| Organ: Eye  |   |   |
| <b>Respiratory or skin sensitization</b>                              |   |   |
| <b>Respiratory sensitization</b>                                      | Knowledge about health hazard is incomplete.  |   |
| <b>Skin sensitization</b>   | Knowledge about health hazard is incomplete.  |   |
| Skin sensitization  |   |   |
| Result: Not sensitization.  |   |   |
| Species: Mouse  |   |   |
| <b>Germ cell mutagenicity</b>   | Knowledge about mutagenicity is incomplete.   |   |
| <b>Carcinogenicity</b>  | Knowledge about carcinogenicity is incomplete.  |   |
| 102 - 170 mg/kg Long-term study                                       |   |   |
| Result: No increase in tumor incidence.                               |   |   |
| Species: Rat  |   |   |
| Test Duration: 2 years  |   |   |
| Epidemiological study of coffee consumption                           |   |   |
| Result: Weak association with bladder cancer.                         |   |   |
| Species: Human  |   |   |
| <b>IARC Monographs. Overall Evaluation of Carcinogenicity</b>         |   |   |
| Caffeine Melting Point Standard (CAS 58-08-2)                         |   | 3 Not classifiable as to carcinogenicity to humans. |
| <b>OSHA Specifically Regulated Substances (29 CFR 1910.1001-1053)</b> |   |   |
| Not listed.   |   |   |
| <b>US. National Toxicology Program (NTP) Report on Carcinogens</b>    |   |   |
| Not listed.   |   |   |
| <b>Reproductive toxicity</b>  | Knowledge about health hazard is incomplete.<br>Caffeine intake in humans does not appear to increase the risk of birth defects. There are conflicting data on whether high daily doses increase the risk of miscarriage or decreased birth weight. |   |
| <b>Specific target organ toxicity - single exposure</b>               | Knowledge about health hazard is incomplete.  |   |
| <b>Specific target organ toxicity - repeated exposure</b>             | Knowledge about health hazard is incomplete.  |   |
| <b>Aspiration hazard</b>  | Based on available data, the classification criteria are not met.   |   |
| <b>Further information</b>  | Pharmacologically active material. Occupational exposure may cause physiological effects.   |   |

## 12. Ecological information

### Ecotoxicity

| Product                                       |      | Species                                     | Test Results        |
|---|------|---|---------------------|
| Caffeine Melting Point Standard (CAS 58-08-2) |      |   |                     |
| Other   | EC50 | Pseudomonas putida                          | 3490 mg/l, 17 hours |
| <b>Aquatic</b>                                |      |   |                     |
| Crustacea                                     | EC50 | Daphnia magna                               | 182 mg/l, 48 hours  |
| Fish  | LC50 | Fathead minnow (Pimephales promelas)        | 151 mg/l, 96 hours  |
|   |      | Ide, silver or golden orfe (Leuciscus idus) | 87 mg/l, 96 hours   |

**Persistence and degradability** Poorly biodegradable.

### Bioaccumulative potential

#### Octanol/water partition coefficient log Kow

-0.091, = Log Pow at 23 °C

**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** Empty containers should be taken to an approved waste handling site for recycling or disposal. Since emptied containers may retain product residue, follow label warnings even after container is emptied.

## 14. Transport information

### DOT

|                                   |                                     |
|-----------------------------------|-------------------------------------|
| <b>UN number</b>                  | UN1544                              |
| <b>UN proper shipping name</b>    | Alkaloids, solid, n.o.s. (Caffeine) |
| <b>Transport hazard class(es)</b> |                                     |
| <b>Class</b>                      | 6.1                                 |
| <b>Subsidiary risk</b>            | -                                   |
| <b>Packing group</b>              | III                                 |
| <b>Packaging exceptions</b>       | 153                                 |
| <b>Packaging non bulk</b>         | 213                                 |
| <b>Packaging bulk</b>             | 240                                 |

### IATA

|                                     |                                     |
|-------------------------------------|-------------------------------------|
| <b>UN number</b>                    | UN1544                              |
| <b>UN proper shipping name</b>      | Alkaloids, solid, n.o.s. (Caffeine) |
| <b>Transport hazard class(es)</b>   |                                     |
| <b>Class</b>                        | 6.1                                 |
| <b>Subsidiary risk</b>              | -                                   |
| <b>Packing group</b>                | III                                 |
| <b>Other information</b>            |                                     |
| <b>Passenger and cargo aircraft</b> | Allowed with restrictions.          |
| <b>Cargo aircraft only</b>          | Allowed with restrictions.          |

**Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code** Not applicable.

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**

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.  
CERCLA/SARA Hazardous Substances - Not applicable.

**Toxic Substances Control Act (TSCA)**

**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.

**OSHA Specifically Regulated Substances (29 CFR 1910.1001-1053)**

Not listed.

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

**SARA 302 Extremely hazardous substance**

Not listed.

**SARA 311/312 Hazardous chemical**

Yes

**Classified hazard categories**

Acute toxicity (any route of exposure)

**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**

| Country(s) or region | Inventory name   | On inventory (yes/no)* |
|----------------------|--|------------------------|
| Australia            | Australian Inventory of Chemical Substances (AICS)                     | Yes                    |
| Canada               | Domestic Substances List (DSL)   | Yes                    |
| Canada               | Non-Domestic Substances List (NDSL)                                    | No                     |
| China                | Inventory of Existing Chemical Substances in China (IECSC)             | Yes                    |
| Europe               | European Inventory of Existing Commercial Chemical Substances (EINECS) | Yes                    |
| Europe               | European List of Notified Chemical Substances (ELINCS)                 | No                     |
| Japan                | Inventory of Existing and New Chemical Substances (ENCS)               | Yes                    |

| Country(s) or region        | Inventory name  | On inventory (yes/no)* |
|-----------------------------|---|------------------------|
| Korea                       | Existing Chemicals List (ECL)                                     | Yes                    |
| New Zealand                 | New Zealand Inventory   | Yes                    |
| Philippines                 | Philippine Inventory of Chemicals and Chemical Substances (PICCS) | Yes                    |
| Taiwan                      | Taiwan Chemical Substance Inventory (TCSI)                        | Yes                    |
| United States & Puerto Rico | Toxic Substances Control Act (TSCA) Inventory                     | Yes                    |

\*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

|                      |   |
|----------------------|---|
| <b>Issue date</b>    | 11-05-2012  |
| <b>Revision date</b> | 05-19-2020  |
| <b>Version #</b>     | 03  |
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