



SAFETY DATA SHEET

1. Identification

Product identifier	Caffeine	
Other means of identification		
Catalog number	1085003	
CAS number	58-08-2	
Synonyms	1,3,7-Trimethylxanthine	
Chemical name	1H-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl-	
Recommended use	For analytical laboratory 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	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
	Acute toxicity, inhalation	Category 4
Environmental hazards	Not classified.	
OSHA defined hazards	Not classified.	
Label elements		



Signal word	Danger	
Hazard statement	Toxic if swallowed. Harmful if inhaled.	
Precautionary statement		
Prevention	Avoid breathing dust. Wash thoroughly after handling. Use only outdoors or in a well-ventilated area.	
Response	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.	
Storage	Store locked up.	
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

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

Information provided in the SDS is not specific to the lot provided. Refer to the label and USP Certificate/Product Information Sheet for the assigned value of a particular lot.

4. First-aid measures

Inhalation	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. Oxygen or artificial respiration if needed. Induce artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Call a physician or poison control center immediately.
Skin contact	Wash off with soap and water. Get medical attention if irritation develops and persists.
Eye contact	Rinse with water. Get medical attention if irritation develops and persists.
Ingestion	Rinse mouth. If vomiting occurs, keep head low so that stomach content doesn't get into the lungs. If ingestion of a large amount does occur, call a poison control center immediately. Do not induce vomiting without advice from poison control center. Get medical attention if symptoms occur.
Most important symptoms/effects, acute and delayed	Central nervous system effects. 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.
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	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	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. For waste disposal, see section 13 of the SDS.
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 materials, 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. 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
-------------------------	------	-------

Caffeine (CAS 58-08-2)	TWA	200 micrograms/m ³
------------------------	-----	-------------------------------

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 USP materials.

9. Physical and chemical properties

Appearance

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

Physical state

Solid.

Form

Crystalline 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

Flammability limit - lower (%)

Not available.

Flammability limit - upper (%)

Not available.

Explosive limit - lower (%)

Not available.

Explosive limit - upper (%)

Not available.

Vapor pressure

15 mm Hg at 89 °C

Vapor density	Not available.
Relative density	Not available.
Solubility(ies)	
Solubility (water)	Sparingly soluble.
Solubility (other)	Chloroform: Freely soluble. Ethanol: Sparingly soluble. Ether: Slightly soluble. 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	
Chemical family	Methylated xanthine.
Molecular formula	C8H10N4O2
Molecular weight	194.19
pH in aqueous solution	5.5 - 6.9 Solution: 1%
Specific gravity	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. Phenols. Tannins. Caustic solutions.
Hazardous decomposition products	NOx. Irritating and/or toxic fumes or gases. Emits toxic fumes under fire conditions.

11. Toxicological information

Information on likely routes of exposure

Inhalation	Harmful if inhaled.
Skin contact	Knowledge about health hazard is incomplete.
Eye contact	Knowledge about health hazard is incomplete.
Ingestion	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 (CAS 58-08-2)		
Oral		
LD50	Rat	192 mg/kg
<u>Acute</u>		
Dermal		
LD50	Rat	> 2000 mg/kg
Inhalation		
LC50	Rat	4.94 mg/l, 4 hours
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
Result: Negative.
Species: Rabbit
Skin irritation
Result: Negative.
Species: Rabbit

Respiratory or skin sensitization

Respiratory sensitization Knowledge about health hazard is incomplete.

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

Local lymph node assay
Result: Non-sensitizing.
Species: Mouse

Germ cell mutagenicity Knowledge about mutagenicity is incomplete.

Carcinogenicity Knowledge about carcinogenicity is incomplete.

102 - 170 mg/kg Carcinogenicity
Result: No increase in tumor incidence.
Species: Rat
Test Duration: 2 years
Carcinogenicity: Epidemiological study of coffee consumption
Result: Weak association with bladder cancer.
Species: Human

IARC Monographs. Overall Evaluation of Carcinogenicity

Caffeine (CAS 58-08-2) 3 Not classifiable as to carcinogenicity to humans.

OSHA Specifically Regulated Substances (29 CFR 1910.1001-1053)

Not listed.

US. National Toxicology Program (NTP) Report on Carcinogens

Not listed.

Reproductive toxicity

Knowledge about health hazard is incomplete.
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.

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

Product		Species	Test Results
Caffeine (CAS 58-08-2)			
Other	EC50	Pseudomonas putida	3490 mg/l, 17 hours
Aquatic			
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 Since emptied containers may retain product residue, follow label warnings even after container is emptied.

14. Transport information

DOT

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

IATA

UN number UN1544
UN proper shipping name Alkaloids, solid, n.o.s. (Caffeine)
Transport hazard class(es)
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 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 This product is a "Hazardous Chemical" as defined by the OSHA Hazard Communication Standard, 29 CFR 1910.1200.

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 Proposition 65**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. For more information go to www.P65Warnings.ca.gov.**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
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

Issue date	12-19-2006
Revision date	12-07-2021
Version #	07

Disclaimer

USP materials are sold for analytical laboratory use only, and NOT for human consumption. The information contained herein is applicable solely to the chemical substance when used for analytical laboratory use and does not necessarily relate to any other use of the substance described, (i.e. at different concentrations, in drug dosage forms, or in bulk quantities). USP materials are intended for use by persons having technical skill and at their own discretion and risk. This information has been developed by USP staff from sources considered reliable but has not been independently verified by the USP. Therefore, the USP Convention cannot guarantee the accuracy of the information in these sources nor should the statements contained herein be considered an official expression. NO REPRESENTATION OR WARRANTY, EXPRESS OR IMPLIED, INCLUDING THE WARRANTIES OF MERCHANTABILITY AND FITNESS FOR A PARTICULAR PURPOSE is made with respect to the information contained herein.