

Theobromine SDS/MSDS (Safety Data Sheet)

1. PRODUCT AND COMPANY IDENTIFICATION

Product identifier

- * Product Name: Theobromine
- * Catalog Number: S2368
- * CAS Number: 83-67-0
- * IUPAC Name: 1H-Purine-2,6-dione, 3,7-dihydro-3,7-dimethyl-

Relevant identified uses and uses advised against

- * Identified uses: For research and development use only; laboratory chemicals; manufacture of substances.
- * Uses advised against: Not for pharmaceutical, household, or other unapproved uses.

Details of the supplier

- * Company: Selleck Chemicals
- * TollFree: +1 877 796-6397
- * Tel: +1 832 582-8158
- * Fax: +1 832 582-8590

Emergency telephone number

- * Emergency phone #: +1 832 582-8158

2. HAZARDS IDENTIFICATION

2.1 GHS classification in accordance with 29 CFR 1910 (OSHA HCS):

- Acute toxicity (oral): Category 4. H302
- Serious eye irritation: Category 2. H319
- Germ cell mutagenicity: Category 2. H341
- Carcinogenicity: Category 2. H351
- Reproductive toxicity: Category 1. H360
- Specific target organ toxicity (single exposure): Category 1. H370

2.2 GHS Label elements, including precautionary statements

Hazard Pictogram(s)



Signal Word

Danger

Hazard statement(s)

- H302: Harmful if swallowed
- H319: Causes serious eye irritation
- H341: Suspected of causing genetic defects
- H351: Suspected of causing cancer
- H360: May damage fertility or the unborn child
- H370: Causes damage to organs

Precautionary statement(s)

None.

Prevention	<p>P203: Obtain, read and follow all safety instructions before use.</p> <p>P260: Do not breathe dust/fume/gas/mist/vapors/spray.</p> <p>P264: Wash hands thoroughly after handling.</p> <p>P264+P265: Wash hands thoroughly after handling. Do not touch eyes.</p> <p>P270: Do not eat, drink or smoke when using this product.</p> <p>P280: Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.</p>
Response	<p>P301+P317: IF SWALLOWED: Get medical help.</p> <p>P305+P351: IF IN EYES: Rinse cautiously with water for several minutes.</p> <p>P308+P316: IF exposed or concerned: Get emergency medical help immediately.</p> <p>P318: if exposed or concerned, get medical advice.</p> <p>P321: Specific treatment (see information on this label and safety datasheet)).</p> <p>P330: Rinse mouth.</p> <p>P337+P317: If eye irritation persists: Get medical help.</p> <p>P338: Remove contact lenses, if present and easy to do. Continue rinsing.</p>
Storage	P405: Store locked up.
Disposal	P501: P501 Dispose of contents/ container to an approved waste disposal plant.

2.3 Other hazards

None.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Product name: Theobromine

CAS Number: 83-67-0

PubChem CID: 5429

Molecular formula: C₇H₈N₄O₂

Molecular weight: 180.16 g/mol

IUPAC name: 3,7-dimethylpurine-2,6-dione

3.2 Mixtures

Not applicable (pure substance).

4. FIRST-AID MEASURES

4.1 Description of first aid measures

Inhalation: INHALATION: IMMEDIATELY leave the contaminated area; take deep breaths of fresh air. If symptoms (such as wheezing, coughing, shortness of breath, or burning in the mouth, throat, or chest) develop, call a physician and be prepared to transport the victim to a hospital. Provide proper respiratory protection to rescuers entering an unknown atmosphere. Whenever possible, Self-Contained Breathing Apparatus (SCBA) should be used; if not available, use a level of protection greater than or equal to t

Skin contact: SKIN: IMMEDIATELY flood affected skin with water while removing and isolating all contaminated clothing. Gently wash all affected skin areas thoroughly with soap and water. If symptoms such as redness or irritation develop, IMMEDIATELY call a physician and be prepared to transport the victim to a hospital for treatment.

Eye contact: EYES: First check the victim for contact lenses and remove if present. Flush victim's eyes with water or normal saline solution for 20 to 30 minutes while simultaneously calling a hospital or poison control center. Do not put any ointments, oils, or medication in the victim's eyes without specific instructions from a physician.

IMMEDIATELY transport the victim after flushing eyes to a hospital even if no symptoms (such as redness or irritation) develop.

Ingestion: INGESTION: DO NOT INDUCE VOMITING. If the victim is conscious and not convulsing, give 1 or 2 glasses of water to dilute the chemical and IMMEDIATELY call a hospital or poison control center. Be prepared to transport the victim to a hospital if advised by a physician. If the victim is convulsing or unconscious, do not give anything by mouth, ensure that the victim's airway is open and lay the victim on his/her side with the head lower than the body. DO NOT INDUCE VOMITING. IMMEDIATELY transport

4.2 Most important symptoms and effects, both acute and delayed

See Section 11 (Toxicological Information).

4.3 Indication of any immediate medical attention and special treatment needed

Treat symptomatically. Contact a poison control center or physician for severe exposure.

5. FIRE-FIGHTING MEASURES

5.1 Extinguishing media

Suitable: Water spray, dry chemical, carbon dioxide (CO₂), alcohol-resistant foam.

Unsuitable: None known.

5.2 Specific hazards arising from the substance or mixture

Fires involving this material can be controlled with a dry chemical, carbon dioxide or Halon extinguisher. (NTP, 1992)

Suitable extinguishing media: Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

Advice for firefighters: Wear self-contained breathing apparatus for firefighting if necessary.

5.3 Advice for firefighters

Wear self-contained breathing apparatus (SCBA) and full protective clothing.

Fight fire from upwind. Cool containers with water spray until fire is extinguished.

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Wear appropriate personal protective equipment (see Section 8).

Avoid breathing dust/vapor. Ensure adequate ventilation.

Evacuate personnel to safe areas. Keep people away from and upwind of spill.

6.2 Environmental precautions

Prevent product from entering drains, waterways, or soil.

Contain spill with inert absorbent material.

6.3 Methods and materials for containment and cleaning up

ACCIDENTAL RELEASE MEASURES: Personal precautions, protective equipment and emergency procedures:

Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate

ventilation. Avoid breathing dust. Environmental precautions: Do not let product enter drains. Methods and materials for containment and cleaning up: Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

SRP: Recycle any unused portion of the material for its approved use or return it to the manufacturer or supplier. Ultimate disposal of the chemical must consider: the material's impact on air quality; potential migration in air, soil or water; effects on animal, aquatic and plant life; and conformance with environmental and public health regulations. If it is possible or reasonable use an alternative chemical product with less inherent propensity for occupational harm/injury/toxicity or environmental contamination.

Product: Offer surplus and non-recyclable solutions to a licensed disposal company; Contaminated packaging: Dispose of as unused product.

ACCIDENTAL RELEASE MEASURES: Personal precautions, protective equipment and emergency procedures: Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Avoid breathing dust. Environmental precautions: Do not let product enter drains. Methods and materials for containment and cleaning up: Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

Precautions for safe handling: Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Provide appropriate exhaust ventilation at places where dust is formed. Normal measures for preventive fire protection.

Appropriate engineering controls: Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

SRP: Local exhaust ventilation should be applied wherever there is an incidence of point source emissions or dispersion of regulated contaminants in the work area. Ventilation control of the contaminant as close to its point of generation is both the most economical and safest method to minimize personnel exposure to airborne contaminants. Ensure that the local ventilation moves the contaminant away from the worker.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

SMALL SPILLS AND LEAKAGE: If you spill this chemical, dampen the solid spill material with 5% ammonium hydroxide, then transfer the dampened material to a suitable container. Use absorbent paper dampened with 5% ammonium hydroxide to pick up any remaining material. Your contaminated clothing and the absorbent paper should be sealed in a vapor-tight plastic bag for eventual disposal. Wash all contaminated surfaces with 5% ammonium hydroxide followed by washing with a soap and water solution. Do not reenter the contaminated area until the Safety Officer (or other responsible person) has verified that the area has been properly cleaned.

STORAGE PRECAUTIONS: You should protect this chemical from light and store this it under ambient temperatures. (NTP, 1992)

Keep container tightly closed in a dry and well-ventilated place. Store under inert gas. Air sensitive.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Store under inert gas. Air sensitive.

Store away from incompatible materials (see Section 10).

[Note: Specific storage temperature not available in public databases. Refer to supplier Certificate of Analysis (COA) for exact storage conditions.]

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Exposure controls

8.1.1 Occupational exposure limits (OEL)

OSHA PEL: Not established.

ACGIH TLV: Not established.

NIOSH REL: Not established.

No occupational exposure limit values are established for this substance.

Use the lowest feasible exposure level (ALARA principle).

8.1.2 Appropriate engineering controls

Use in a well-ventilated area. Chemical fume hood recommended for powder handling.

8.2 Individual protection measures

8.2.1 Eye/face protection

Wear chemical safety goggles.

8.2.2 Skin protection

Wear protective gloves. Recommended material: Nitrile rubber.

Wear suitable protective clothing (lab coat).

8.2.3 Respiratory protection

Respiratory protection usually not required under normal use with adequate ventilation.

Use N95 respirator for large-scale powder handling.

8.2.4 Thermal hazards

Not applicable.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

- a) Appearance: Theobromine is an odorless white crystalline powder. Bitter taste. pH (saturated solution in water): 5.5-7. (NTP, 1992)
- b) Odor: No data available
- c) Odor threshold: No data available
- d) pH: No data available
- e) Melting point/freezing point: 675 °F (NTP, 1992)
- f) Initial boiling point and boiling range: Sublimes at 554-563 °F (NTP, 1992)
- g) Flash point: No data available
- h) Evaporation rate: No data available
- i) Flammability (solid, gas): No data available
- j) Upper/lower flammability or explosive limits: No data available
- k) Vapor pressure: No data available
- l) Vapor density: No data available
- m) Relative density: 1.522 g/cu cm at 20 °C; relative density: 1.522 at 20 °C
- n) Water solubility: less than 1 mg/mL at 64 °F (NTP, 1992)
- o) Partition coefficient: n-octanol/water: Log P (n-octanol/water): -0.8
- p) Auto-ignition temperature: No data available
- q) Decomposition temperature: No data available
- r) Viscosity: No data available

s) Explosive properties: No data available

t) Oxidizing properties: No data available

9.2 Other information

Topological Polar Surface Area (TPSA): 67.2 Å²

Complexity: 267

10. STABILITY AND REACTIVITY

10.1 Reactivity

No specific reactivity hazards identified under normal handling conditions.

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

No hazardous reactions under normal conditions.

10.4 Conditions to avoid

Avoid heat, sparks, open flames, direct sunlight, and moisture.

Avoid strong oxidizing agents, strong acids, and strong bases.

10.5 Incompatible materials

Incompatible materials: Strong oxidizing agents

10.6 Hazardous decomposition products

Thermal decomposition may produce: Carbon monoxide (CO), Carbon dioxide (CO₂), Nitrogen oxides (NO_x).

See also Section 5 (Fire-fighting measures) for combustion products.

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity:

No acute toxicity data available.

Skin corrosion/irritation:

No data available.

Serious eye damage/eye irritation:

Causes serious eye irritation (H319).

Respiratory or skin sensitization:

No data available.

Germ cell mutagenicity:

Suspected of causing genetic defects (H341).

Carcinogenicity:

Suspected of causing cancer (H351).

Reproductive toxicity:

May damage fertility or the unborn child (H360).

Specific target organ toxicity (single exposure):

H370

Specific target organ toxicity (repeated exposure):

No data available.

Aspiration hazard:

No data available.

11.2 Additional information

Carcinogen classification:

Theobromine

Group 3: Not classifiable as to its carcinogenicity to humans

Volume 51: (1991) Coffee, Tea, Mate, Methylxanthines and Methylglyoxal

1991

1990

Data source: Hazardous Substances Data Bank (HSDB) via PubChem.

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Theobromine is a breakdown metabolite of caffeine which may result in its release to the environment through various waste streams. Its former production and use as a medication in human and veterinary medicine as well have may resulted in its release to the environment through various waste streams. Theobromine is the principal alkaloid of the cacao bean and occurs in fresh tea leaves and coffee. If released to air, an estimated vapor pressure of 1.1×10^{-11} mm Hg at 25 °C indicates theobromine will exist solely in the particulate phase in the atmosphere. Particulate-phase theobromine will be removed from the atmosphere by wet and dry deposition. Theobromine absorbs UV light at wavelengths of 272 nm and, therefore, is not expected to be susceptible to direct photolysis by sunlight. If released to soil, theobromine is expected to have very high mobility based upon an estimated Koc of 10. Volatilization from moist soil surfaces is not expected to be an important fate process based upon an estimated Henry's Law constant of 1.6×10^{-11} atm-cu m/mole. Theobromine is not expected to volatilize from dry soil surfaces based upon its vapor pressure. Using an acclimated sewage sludge inoculum, theobromine reached 100% of its Theoretical BOD in 28 days, suggesting that biodegradation may be an important environmental fate process in soil and water previously exposed to this compound. If released into water, theobromine is not expected to adsorb to suspended solids and sediment based upon t

12.2 Persistence and degradability

No data available.

12.3 Bioaccumulative potential

Log P (n-octanol/water): -0.8

Low potential for bioaccumulation (Log P < 3).

12.4 Mobility in soil

No data available.

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available.

12.6 Other adverse effects

No other adverse ecological effects identified.

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Waste Treatment Methods: Waste material must be disposed of in accordance with national and local regulations. Leave chemicals in original containers and do not mix with other waste. Handle uncleaned containers in the same manner as the product itself.

14. TRANSPORT INFORMATION

14.1 UN number

Not regulated as dangerous goods (research quantities typically exempt).

14.2 UN proper shipping name

Not subject to transport regulations (small quantities for research use).

14.3 Transport hazard class(es)

Not classified as dangerous goods for transport (research quantities).

14.4 Packing group

Not applicable (not regulated as dangerous goods in typical research quantities).

14.5 Environmental hazards

Marine pollutant: No (not classified as environmentally hazardous per GHS).

14.6 Special precautions for user

Transport in original packaging. Ensure containers are tightly sealed.

For bulk or commercial quantities, consult applicable transport regulations (DOT, IATA, IMDG).

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

Not applicable.

15. REGULATORY INFORMATION

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

US EPA / TSCA: Subject to EPA TSCA regulations

EU ECHA / REACH: Registered (REACH Active)

SARA 302 Components:

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components:

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards:

Acute (short-term) health hazard

Chronic (long-term) health hazard

Massachusetts Right To Know Components:

This material contains components subject to the Massachusetts Right to Know Act. See Section 2 for hazard classification.

Pennsylvania Right To Know Components:

This material contains components subject to the Pennsylvania Right to Know Act. See Section 2 for hazard classification.

New Jersey Right To Know Components:

This material contains components subject to the New Jersey Right to Know Act. See Section 2 for hazard classification.

California Prop. 65 Components:

This product does not contain any chemicals known to the State of California to cause cancer, birth defects, or any other reproductive harm.

Other regulatory listings:

- The Australian Inventory of Industrial Chemicals: Chemical: 1H-Purine-2,6-dione, 3,7-dihydro-3,7-dimethyl-
- EFSA Legal Basis: Commission Regulation (EC) No 1565/2000 (Repealed by Com. Implementing Reg. (EU) No 872/2012)
- FDA Requirements: Drug products containing certain active ingredients offered over-the-counter (OTC) for certain uses. A number of active ingredients have been present in OTC drug products for various uses, as described below. However, based on evidence currently available, there are inadequate data to establish gen

15.2 Chemical safety assessment

A chemical safety assessment has not been carried out for this substance.

For research-use-only compounds, no CSA is required under REACH Annex I.

16. OTHER INFORMATION

Revision Date: 2026/09/08

Further Information: The information provided is believed to be correct but is not exhaustive and should be used only as a guideline based on current knowledge. It does not represent a guarantee of the properties of the product. Selleck Chemicals Corporation and its Affiliates shall not be held liable for any damage resulting from handling or contact with the product.