

Mercaptopurine (6-MP) SDS/MSDS (Safety Data Sheet)

1. PRODUCT AND COMPANY IDENTIFICATION

Product identifier

* Product Name: Mercaptopurine (6-MP)

* Catalog Number: S1305

* CAS Number: 50-44-2

* IUPAC Name: 3H-purine-6(7H)-thione

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 3. H301

Acute toxicity (oral): Category 4. H302

Skin irritation: Category 2. H315

Serious eye irritation: Category 2. H319

Specific target organ toxicity (single exposure): Category 3. H335

Germ cell mutagenicity: Category 1. H340

Reproductive toxicity: Category 1. H360

Reproductive toxicity: Category 2. H361

Specific target organ toxicity (single exposure): Category 1. H370

Specific target organ toxicity (repeated exposure): Category 1. H372

2.2 GHS Label elements, including precautionary statements

Hazard Pictogram(s)



Signal Word

Danger

Hazard statement(s)	H301: Toxic if swallowed H302: Harmful if swallowed H315: Causes skin irritation H319: Causes serious eye irritation H335: May cause respiratory irritation H340: May cause genetic defects H360: May damage fertility or the unborn child H361: Suspected of damaging fertility or the unborn child H370: Causes damage to organs H372: Causes damage to organs through prolonged or repeated exposure
Precautionary statement(s)	None.
Prevention	P203: Obtain, read and follow all safety instructions before use. P260: Do not breathe dust/fume/gas/mist/vapors/spray. P261: Avoid breathing dust/fume/gas/mist/vapors/spray. P264: Wash hands thoroughly after handling. P264+P265: Wash hands thoroughly after handling. Do not touch eyes. P270: Do not eat, drink or smoke when using this product. P271: Use only outdoors or in a well-ventilated area. P280: Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.
Response	P301+P316: IF SWALLOWED: Get emergency medical help immediately. P301+P317: IF SWALLOWED: Get medical help. P302+P352: IF ON SKIN: wash with plenty of water. P304+P340: IF INHALED: Remove person to fresh air and keep comfortable for breathing. P305+P351: IF IN EYES: Rinse cautiously with water for several minutes. P308+P316: IF exposed or concerned: Get emergency medical help immediately. P318: if exposed or concerned, get medical advice. P319: Get medical help if you feel unwell. P321: Specific treatment (see information on this label and safety datasheet)). P330: Rinse mouth. P332+P317: If skin irritation occurs: Get medical help. P337+P317: If eye irritation persists: Get medical help. P338: Remove contact lenses, if present and easy to do. Continue rinsing. P362+P364: Take off contaminated clothing and wash it before reuse.
Storage	P403+P233: Store in a well-ventilated place. Keep container tightly closed. 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: Mercaptopurine (6-MP)

CAS Number: 50-44-2

PubChem CID: 667490

Molecular formula: C₅H₄N₄S

Molecular weight: 152.18 g/mol

IUPAC name: 3,7-dihydropurine-6-thione

3.2 Mixtures

Not applicable (pure substance).

4. FIRST-AID MEASURES

4.1 Description of first aid measures

Inhalation: Move to fresh air. Keep at rest in a position comfortable for breathing. Seek medical attention if symptoms persist.

Skin contact: Wash with plenty of soap and water. Remove contaminated clothing. Seek medical attention if irritation develops.

Eye contact: Rinse cautiously with water for several minutes. Remove contact lenses if present and easy to do. Continue rinsing. Seek medical attention.

Ingestion: Rinse mouth. Do NOT induce vomiting unless directed by medical personnel. Seek medical attention.

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

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

/6-Mercaptopurine monohydrate/

Advice for firefighters: Wear self contained breathing apparatus for fire fighting if necessary. /6-Mercaptopurine monohydrate/

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.

WARNING: Highly toxic — only trained personnel should handle spills.

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. Evacuate personnel to safe areas. 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. /6-Mercaptopurine monohydrate/ SRP: Expired or waste pharmaceuticals shall carefully take into consideration applicable DEA, EPA, and FDA regulations. It is not appropriate to dispose by flushing the pharmaceutical down the toilet or discarding to trash. If possible return the pharmaceutical to the manufacturer for proper disposal being careful to properly label and securely package the material. Alternatively, the waste pharmaceutical shall be labeled, securely packaged and transported by a state licensed medical waste contractor to dispose by burial in a licensed hazardous or toxic waste landfill or incinerator.

Product: Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber; Contaminated packaging: Dispose of as unused product. /6-Mercaptopurine monohydrate/

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. Evacuate personnel to safe areas. Avoid breathing dust. Environmental precautions: Do not let product enter drains. /6-Mercaptopurine monohydrate/

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. /6-Mercaptopurine monohydrate/

Appropriate engineering controls: Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday. /6-Mercaptopurine monohydrate/

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. /6-Mercaptopurine monohydrate/

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

Store at 20 deg to 25 °C (68 deg to 77 °F). Store in a dry place.

Keep container tightly closed in a dry and well-ventilated place. /6-Mercaptopurine monohydrate/

7.2 Conditions for safe storage, including any incompatibilities

Store at 20 deg to 25 °C (68 deg to 77 °F). Store in a dry place.

Keep container tightly closed in a dry and well-ventilated place. /6-Mercaptopurine monohydrate/

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 only in a chemical fume hood or with local exhaust ventilation.

Ensure adequate ventilation to keep airborne concentrations below exposure limits.

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

Use NIOSH-approved dust/mist respirator (N95 or higher) if ventilation is inadequate.

8.2.4 Thermal hazards

Not applicable.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a) Appearance: Solid

b) Odor: Nearly odorless

c) Odor threshold: No data available

d) pH: No data available

e) Melting point/freezing point: 308 °C (decomposes)

f) Initial boiling point and boiling range: No data available

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: No data available
- n) Water solubility: In water, 6848 mg/L at 30 °C
- o) Partition coefficient: n-octanol/water: Log P: 0
- 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): 85.2 Å²

Complexity: 190

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, strong bases, strong acids. /6-Mercaptopurine monohydrate/

10.6 Hazardous decomposition products

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

Causes skin irritation (H315).

Serious eye damage/eye irritation:

Causes serious eye irritation (H319).

Respiratory or skin sensitization:

No data available.

Germ cell mutagenicity:

May cause genetic defects (H340).

Carcinogenicity:

No data available.

Reproductive toxicity:

May damage fertility or the unborn child (H360).

Specific target organ toxicity (single exposure):

H370, H372

Specific target organ toxicity (repeated exposure):

No data available.

Aspiration hazard:

No data available.

11.2 Additional information

Carcinogen classification:

6-Mercaptopurine

Group 3: Not classifiable as to its carcinogenicity to humans

Volume 26: (1981) Some Antineoplastic and Immunosuppressive Agents

Volume Sup 7: Overall Evaluations of Carcinogenicity: An Updating of IARC Monographs Volumes 1 to 42, 1987; 440 pages; ISBN 92-832-1411-0 (out of print)

1987

1987

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

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Mercaptopurine's production and administration as a medication may result in its release to the environment through various waste streams. If released to air, an estimated vapor pressure of 1.3×10^{-8} mm Hg at 25 °C indicates mercaptopurine will exist in both the vapor and particulate phases. Vapor-phase mercaptopurine will be degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 0.05 days. Particulate-phase mercaptopurine will be removed from the atmosphere by wet and dry deposition. Mercaptopurine absorbs UV light at wavelengths >290 nm and, therefore, may be susceptible to direct photolysis by sunlight. If released to soil, mercaptopurine is expected to have high mobility based upon an estimated Koc of 89. Volatilization from moist soil surfaces is not expected to be an important fate process based upon an estimated Henry's Law constant of 7.5×10^{-10} atm-cu m/mole. Mercaptopurine is not expected to volatilize from dry soil surfaces based upon its vapor pressure. Biodegradation data in soil or water were not available. If released into water, mercaptopurine is not expected to adsorb to suspended solids and sediment based upon the estimated Koc. Volatilization from water surfaces is not expected to be an important fate process based upon this compound's estimated Henry's Law constant. An estimated BCF of 3 suggests the potential for bioconcentration in aquatic organisms is low. Hydrolysi

12.2 Persistence and degradability

No data available.

12.3 Bioaccumulative potential

No data available.

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: Not available in public databases.

EU ECHA / REACH: Not available in public databases.

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:

- California Safe Cosmetics Program (CSCP) Reportable Ingredient: Hazard Traits - Developmental Toxicity Authoritative List - Prop 65 Report - regardless of intended function of ingredient in the product
- FDA Requirements: The Approved Drug Products with Therapeutic Equivalence Evaluations identifies currently marketed prescription drug products, including mercaptopurine, approved on the basis of safety and effectiveness by FDA under sections 505 of the Federal Food, Drug, and Cosmetic Act.

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.