

Allopurinol SDS/MSDS (Safety Data Sheet)

1. PRODUCT AND COMPANY IDENTIFICATION

Product identifier

- * Product Name: Allopurinol
- * Catalog Number: S1630
- * CAS Number: 315-30-0
- * IUPAC Name: 1,2-dihydropyrazolo[3,4-d]pyrimidin-4-one

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
- Skin sensitization: Category 1. H317

2.2 GHS Label elements, including precautionary statements

Hazard Pictogram(s)



Signal Word

Danger

Hazard statement(s)

H301: Toxic if swallowed
H317: May cause an allergic skin reaction

Precautionary statement(s)

None.

Prevention

P261: Avoid breathing dust/fume/gas/mist/vapors/spray.
P264: Wash hands thoroughly after handling.
P270: Do not eat, drink or smoke when using this product.
P272: Contaminated work clothing should not be allowed out of the workplace.
P280: Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.

Response	<p>P301+P316: IF SWALLOWED: Get emergency medical help immediately.</p> <p>P302+P352: IF ON SKIN: wash with plenty of water.</p> <p>P321: Specific treatment (see information on this label and safety datasheet)).</p> <p>P330: Rinse mouth.</p> <p>P333+P317: If skin irritation or rash occurs: Get medical help.</p> <p>P362+P364: Take off contaminated clothing and wash it before reuse.</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: Allopurinol

CAS Number: 315-30-0

PubChem CID: 135401907

Molecular formula: C₅H₄N₄O

Molecular weight: 136.11 g/mol

IUPAC name: 1,5-dihydropyrazolo[5,4-d]pyrimidin-4-one

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. If symptoms (such as redness or irritation) develop, immediately transport the victim to a hospital.

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)

Water spray, dry chemical, carbon dioxide, or foam as appropriate for surrounding fire and materials.

As with all fires, evacuate personnel to a safe area. Firefighters should use self-contained breathing equipment and protective clothing.

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

Excerpt from ERG Guide 154 [Substances - Toxic and/or Corrosive (Non-Combustible)]:

IMMEDIATE PRECAUTIONARY MEASURE: Isolate spill or leak area in all directions for at least 50 meters (150 feet) for liquids and at least 25 meters (75 feet) for solids.

SPILL: Increase the immediate precautionary measure distance, in the downwind direction, as necessary.

FIRE: If tank, rail tank car or highway tank is involved in a fire, ISOLATE for 800 meters (1/2 mile) in all directions; also, consider initial evacuation for 800 meters (1/2 mile) in all directions. (ERG, 2024)

Wipe up spillage or collect spillage using a high- efficiency vacuum cleaner. Avoid breathing dust. Place spillage in appropriately labeled container for disposal. Wash spill site.

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.

SRP: At the time of review, regulatory criteria for small quantity disposal are subject to significant revision, however, household quantities of waste pharmaceuticals may be managed as follows: Mix with wet cat litter or coffee grounds, double bag in plastic, discard in trash.

This material is assumed to be combustible. As with all dry powders, it is advisable to ground mechanical equipment in contact with dry material to dissipate the potential buildup of static electricity.

As a general rule, when handling USP Reference Standards avoid all contact and inhalation of dust, mists, and/or vapors associated with the material. Wash thoroughly after handling.

/Use/ safety glasses or goggles /and/ protect exposed skin.

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 store this material in a refrigerator. (NTP, 1992)

Store in tight container as defined in the USP-NF. This material should be handled and stored per label instructions to ensure product integrity.

Allopurinol tablets should be stored in well-closed containers at 15-30 °C. Commercially available allopurinol sodium lyophilized powder for injection should be stored at a controlled room temperature of 25 °C, but may be exposed to temperatures ranging from 15-30 °C. Following reconstitution of allopurinol sodium for injection with sterile water for injection, the solutions contain approximately 20 mg/mL and should be further diluted with 0.9% sodium chloride injection or 5% dextrose injection. These further diluted allopurinol sodium solutions, containing no more than 6 mg/mL, should be stored at 20- 25 °C and should be used within 10 hours of reconstitution. Reconstituted and/or diluted solutions should not be refrigerated.

An oral suspension of allopurinol containing 20 mg/mL has been prepared extemporaneously from the commercially available tablets. The tablets were crushed, mixed with a volume of suspending agent (Cologel) equal to one-third the final volume, and then the suspension was brought to the final volume with a 2:1 mixture of simple syrup and wild cherry syrup. The resulting suspension was stable for at least 14 days when stored in an amber glass bottle at room temperature or 5 °C.

7.2 Conditions for safe storage, including any incompatibilities

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An oral suspension of allopurinol containing 20 mg/mL has been prepared extemporaneously from the commercially available tablets. The tablets were crushed, mixed with a volume of suspending agent (Cologel) equal to one-third

the final volume, and then the suspension was brought to the final volume with a 2:1 mixture of simple syrup and wild cherry syrup. The resulting suspension was stable for at least 14 days when stored in an amber glass bottle at room temperature or 5 °C.

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 safety glasses with side shields.

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: 4-hydroxypyrazolo(3,4-d)pyrimidine is an odorless tasteless white microcrystalline powder. (NTP, 1992)

b) Odor: SLIGHT

c) Odor threshold: No data available

d) pH: No data available

e) Melting point/freezing point: greater than 662 °F (NTP, 1992)

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: less than 1 mg/mL at 64 °F (NTP, 1992)
- o) Partition coefficient: n-octanol/water: Log P (n-octanol/water): -0.7
- 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): 70.1 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 with/ strong oxidizing agents.

Allopurinol sodium injection has been reported to be incompatible with various drugs (eg, sodium bicarbonate), but the compatibility depends on several factors (eg, concentrations of the drugs, resulting pH, temperature). Specialized references should be consulted for specific compatibility information.

Drugs that are physically incompatible in solution with (allopurinol sodium) for Injection Amikacin sulfate, Hydroxyzine HCl, Amphoterecin, Bldarubicin HCl, Carmustine/mipenem-cilastatin sodium, Cefotaxime sodium, Mechlorethamine HCl, Chlorpromazine HCl, Meperidine HCl, Cimetidine HCl, Metoclopramide HCl, Clindamycin phosphate, Methylprednisolone sodium succinate, Cytarabine, Minocycline HCl Dacarbazine, Nalbuphine HCl, Daunorubicin HCl, Netilmicin sulfate, Diphenhydramine HCl, Ondansetron HCl, Doxorubicin HCl, Prochlorperazine edisylate, Doxycycline hyclate, Promethazine HCl, Droperidol, Sodium bicarbonate, Floxuridine, Streptozocin, Gentamicin sulfate, Tobramycin sulfate, Haloperidol lactate, and Vinorelbine tartrate

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:

No data available.

Respiratory or skin sensitization:

May cause an allergic skin reaction (H317).

Germ cell mutagenicity:

No data available.

Carcinogenicity:

No data available.

Reproductive toxicity:

No data available.

Specific target organ toxicity (single exposure):

No data available.

Specific target organ toxicity (repeated exposure):

No data available.

Aspiration hazard:

No data available.

11.2 Additional information

Carcinogen classification:

No indication of carcinogenicity to humans (not listed by IARC).

Exposure routes:

Approximately 80-90% absorbed from the gastrointestinal tract.

Signs and symptoms of exposure:

LD₅₀=214 mg/kg (in mice)

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

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Allopurinol's production and use as a medication may result in its release to the environment through various waste streams. If released to air, an estimated vapor pressure of 1.2×10^{-8} mm Hg at 25 °C indicates allopurinol will exist in both the vapor and particulate phases in the atmosphere. Vapor-phase allopurinol 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 2 hrs. Particulate-phase allopurinol will be removed from the atmosphere by wet or dry deposition. Allopurinol contains chromophores that absorb at wavelengths >290 nm and therefore may be susceptible to direct photolysis by sunlight. If released to soil, allopurinol is expected to have high mobility based upon an estimated Koc of 71. Volatilization from moist soil surfaces is not expected to be an important fate process based upon an estimated Henry's Law constant of 2.0×10^{-14} atm-cu m/mole. Biodegradation data were not available. If released into water, allopurinol 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. Hydrolysis is not expected to be an important environmental fate process since this compound lacks functional groups that hydroly

12.2 Persistence and degradability

No data available.

12.3 Bioaccumulative potential

Log P (n-octanol/water): -0.7

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).

DOT label: Poison

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: 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

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:

- FDA Requirements: The Approved Drug Products with Therapeutic Equivalence Evaluations List identifies currently marketed prescription drug products, including allopurinol, 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.