

Aminopterin SDS/MSDS (Safety Data Sheet)

1. PRODUCT AND COMPANY IDENTIFICATION

Product identifier

* Product Name: Aminopterin

* Catalog Number: E1003

* CAS Number: 54-62-6

* IUPAC Name: L-Glutamic acid, N-[4-[[[(2,4-diamino-6-pteridiny]methyl]amino]benzoyl]-

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 1. H300

Reproductive toxicity: Category 1. H360

2.2 GHS Label elements, including precautionary statements

Hazard Pictogram(s)



Signal Word

Danger

Hazard statement(s)

H300: Fatal if swallowed

H360: May damage fertility or the unborn child

Precautionary statement(s)

None.

Prevention

P203: Obtain, read and follow all safety instructions before use.

P264: Wash hands thoroughly after handling.

P270: Do not eat, drink or smoke when using this product.

P280: Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.

Response	P301+P316: IF SWALLOWED: Get emergency medical help immediately. P318: if exposed or concerned, get medical advice. P321: Specific treatment (see information on this label and safety datasheet)). P330: Rinse mouth.
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: Aminopterin

CAS Number: 54-62-6

PubChem CID: 169371

Molecular formula: C₁₉H₂₀N₈O₅

Molecular weight: 440.4 g/mol

IUPAC name: (2S)-2-[[4-[(2,4-diaminopteridin-6-yl)methylamino]benzoyl]amino]pentanedioic acid

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

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

SMALL FIRE: Dry chemical, CO₂ or water spray.

LARGE FIRE: Dry chemical, CO₂, alcohol-resistant foam or water spray. If it can be done safely, move undamaged containers away from the area around the fire. Dike runoff from fire control for later disposal.

FIRE INVOLVING TANKS, RAIL TANK CARS OR HIGHWAY TANKS: Fight fire from maximum distance or use unmanned master stream devices or monitor nozzles. Do not get water inside containers. Cool containers with flooding quantities of water until well after fire is out. Withdraw immediately in case of rising sound from venting safety devices or discoloration of tank. ALWAYS stay away from tanks in direct contact with flames. (ERG, 2024)

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)

SRP: The most favorable course of action is to use an alternative chemical product with less inherent propensity for occupational exposure or environmental contamination. 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 soil or water; effects on animal, aquatic, and plant life; and conformance with environmental and public health regulations.

SRP: At the time of review, criteria for land treatment or burial (sanitary landfill) disposal practices are subject to significant revision. Prior to implementing land disposal of waste residue (including waste sludge), consult with environmental regulatory agencies for guidance on acceptable disposal practices.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

(Non-Specific -- Pesticide, Solid, n.o.s.) Do not touch spilled material; stop leak if you can do so without risk. Use water spray to reduce vapors.

Small spills: absorb with sand or other noncombustible absorbent material and place into containers for later disposal.

Small dry spills: with clean shovel place material into clean, dry container and cover; move containers from spill area.

Large spills: dike far ahead of spill for later disposal. (EPA, 1998)

7.2 Conditions for safe storage, including any incompatibilities

Store in a cool, dry, well-ventilated area. Keep container tightly closed.

Store away from incompatible materials (see Section 10).

Protect from light and moisture.

Recommended storage (industry convention for research compounds): -20°C for long-term storage; 2-8°C for short-term use and transport.

[Note: This is a general industry recommendation. Always verify exact storage conditions with the supplier Certificate of Analysis (COA).]

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: Clusters of yellow needles. Used as a rodenticide, medicine and rodenticide. Not registered as a rodenticide in the U.S. (EPA, 1998)

b) Odor: No data available

- c) Odor threshold: No data available
- d) pH: No data available
- e) Melting point/freezing point: No data available
- 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: 2.3X10⁻¹⁹ mg Hg at 25 °C /Estimated/
- l) Vapor density: No data available
- m) Relative density: No data available
- n) Water solubility: 3.0X10³ mg/L
- o) Partition coefficient: n-octanol/water: Log P (n-octanol/water): -2
- 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): 219 Å²

Complexity: 674

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

Strong oxidizing agents, strong acids, strong bases.

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:

No data available.

Germ cell mutagenicity:

No data available.

Carcinogenicity:

No data available.

Reproductive toxicity:

May damage fertility or the unborn child (H360).

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).

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

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Aminopterin's former production and use as a research drug for the treatment of leukemias may have resulted in its release to the environment through various waste streams; its former use as a rodenticide resulted in its direct release to the environment. If released to air, an estimated vapor pressure of 2.3×10^{-19} mm Hg at 25 °C indicates aminopterin will exist solely in the particulate phase in the ambient atmosphere. Particulate-phase aminopterin will be removed from the atmosphere by wet and dry deposition. Aminopterin absorbs UV light >290 nm; therefore, on soil surfaces, aminopterin may be susceptible to photolysis. If released to soil, aminopterin is expected to have low mobility based upon an estimated Koc of 650. A measured pKa of one of the carboxylic acid moieties of aminopterin is 5.5, indicates that this compound will primarily exist in anion form in the environment and anions do not volatilize from moist soil or water surfaces and generally do not adsorb more strongly to suspended solids and sediment than their neutral counterparts. The estimated pKa values for the carboxylic acid moieties of aminopterin are 3.5 and 4.3, indicating that this compound will primarily exist in anion form and anions generally do not adsorb more strongly to organic carbon and clay than their neutral counterparts. Aminopterin is not expected to volatilize from dry soil surfaces based upon its vapor pressure. If released into water, aminopterin is expected to adsorb to suspended solids

12.2 Persistence and degradability

No data available.

12.3 Bioaccumulative potential

Log P (n-octanol/water): -2

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

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; Reproductive Toxicity Authoritative List - Prop 65 Report - regardless of intended function of ingredient in the product
- New Jersey Worker and Community Right to Know Act: The New Jersey Worker and Community Right to Know Act requires public and private employers to provide information about hazardous substances at their workplaces. (N.J.S.A. 34:5A-1 et. seq.)
- CERCLA Reportable Quantities: Releases of CERCLA hazardous substances are subject to the release reporting requirement of CERCLA section 103, codified at 40 CFR part 302, in addition to the requirements of 40 CFR part 355. Aminopterin is an extremely hazardous substance (EHS) subject to reporting requirements when stored in amount

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.