3-Amino-1,2,4-triazole (3-AT) SDS/MSDS (Safety Data Sheet)

1. PRODUCT AND COMPANY IDENTIFICATION

Product identifier

* Product Name: 3-Amino-1,2,4-triazole (3-AT)
* Catalog Number: S5977
* CAS Number: 61-82-5
* IUPAC Name: 1H-1,2,4-Triazol-5-amine

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
Skin irritation: Category 3. H316
Skin sensitization: Category 1. H317
Eye irritation: Category 2. H320
Reproductive toxicity: Category 2. H361
Specific target organ toxicity (repeated exposure): Category 1. H372
Specific target organ toxicity (repeated exposure): Category 2. H373
Chronic aquatic toxicity: Category 2. H411

2.2 GHS Label elements, including precautionary statements

Hazard Pictogram(s)



Signal Word Danger

Hazard statement(s)	H302: Harmful if swallowed H316: Causes mild skin irritation H317: May cause an allergic skin reaction H320: Causes eye irritation H361: Suspected of damaging fertility or the unborn child H372: Causes damage to organs through prolonged or repeated exposure H373: May causes damage to organs through prolonged or repeated exposure H411: Toxic to aquatic life with long lasting effects
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. P272: Contaminated work clothing should not be allowed out of the workplace. P273: Avoid release to the environment. P280: Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.
Response	P301+P317: IF SWALLOWED: Get medical help. P302+P352: IF ON SKIN: wash with plenty of water. P305+P351: IF IN EYES: Rinse cautiously with water for several minutes. 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. P333+P317: If skin irritation or rash 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. P391: Collect spillage.
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: 3-Amino-1,2,4-triazole (3-AT)

CAS Number: 61-82-5

PubChem CID: 1639

Molecular formula: C2H4N4

Molecular weight: 84.08 g/mol

IUPAC name: 1H-1,2,4-triazol-5-amine

3.2 Mixtures

Not applicable (pure substance).

4. FIRST-AID MEASURES

4.1 Description of first aid measures

Inhalation: Fresh air, rest.

Skin contact: Remove contaminated clothes. Rinse skin with plenty of water or shower.

Eye contact: First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

Ingestion: Rinse mouth. Refer for 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

Fires involving this chemical can be controlled with a dry chemical, carbon dioxide or Halon extinguisher. A water spray may also be used. (NTP, 1992)

Use water spray, foam, powder, carbon dioxide.

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

Excerpt from ERG Guide 171 [Substances (Low to Moderate Hazard)]:

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)

Personal protection: particulate filter respirator adapted to the airborne concentration of the substance. Do NOT let this chemical enter the environment. Sweep spilled substance into covered sealable, plastic containers. If appropriate, moisten first to prevent dusting. Carefully collect remainder. Then store and dispose of according to local regulations.

PRECAUTIONS FOR "CARCINOGENS": A high-efficiency particulate arrestor (HEPA) or charcoal filters can be used to minimize amt of carcinogen in exhausted air ventilated safety cabinets, lab hoods, glove boxes or animal rooms ... Filter housing that is designed so that used filters can be transferred into plastic bag without contaminating maintenance staff is avail commercially. Filters should be placed in plastic bags immediately after removal ... . The plastic bag should be sealed immediately ... . The sealed bag should be labelled properly ... . Waste liquids ... should be placed or collected in proper containers for disposal. The lid should be secured & the bottles properly labelled. Once filled, bottles should be placed in plastic bags, so that outer surface ... is not contaminated ... . The plastic bag should also be sealed & labelled. ... Broken glassware ... should be decontaminated by solvent extraction, by chemical destruction, or in specially designed incinerators. /Chemical Carcinogens/

If a spill occurs, clean it up promptly. Don't wash it away. Instead, sprinkle the spill with sawdust, vermiculite, or kitty litter. Sweep it into a plastic garbage bag, and dispose of it as directed on the pesticide product label.

After Applying a Pesticide, Indoors or Outdoors. To remove pesticide residues, use a bucket to rinse tools or equipment three times, including any containers or utensils that you used when mixing the pesticide. Then pour the rinsewater into the pesticide sprayer and reuse the solution by applying it according to the pesticide product label directions. After applying any pesticide wash your hands and any other parts of your body that may have come in contact with the pesticide..To prevent tracking pesticides inside, remove or rinse your boots or shoes before entering your home. Wash any clothes that have been exposed to a lot of pesticide separately from your regular wash.

[40 CFR 240-280, 300-306, 702-799 (7/1/2005)] Generators of waste (equal to or greater than 100 kg/mo) containing this contaminant, EPA hazardous waste number U011, must conform with USEPA regulations in storage, transportation, treatment and disposal of waste.

Generators of waste (equal to or greater than 100 kg/mo) containing this contaminant, EPA hazardous waste number U011, must conform with USEPA regulations in storage, transportation, treatment and disposal of waste.

A potential candidate for rotary kiln incineration at a temperature range of 820 to 1,600 °C and residence times of seconds for liquids and gases, and hours for solids. A potential candidate for fluidized bed incineration at a temperature range of 450 to 980 °C and residence times of seconds for liquids and gases, and longer for solids.

The following wastewater treatment technologies have been investigated for aminotriazole: Concentraction process: Biological treatment.

For more Disposal Methods (Complete) data for AMITROLE (11 total), please visit the HSDB record page.

PRECAUTIONS FOR "CARCINOGENS": Smoking, drinking, eating, storage of food or of food & beverage containers or utensils, & the application of cosmetics should be prohibited in any laboratory. All personnel should remove gloves, if worn, after completion of procedures in which carcinogens have been used. They should ... wash ... hands, preferably using dispensers of liq detergent, & rinse ... thoroughly. Consideration should be given to appropriate methods for cleaning the skin, depending on nature of the contaminant. No standard procedure can be recommended, but the use of organic solvents should be avoided. Safety pipettes should be used for all pipetting. /Chemical Carcinogens/

PRECAUTIONS FOR "CARCINOGENS": In animal laboratory, personnel should remove their outdoor clothes & wear protective suits (preferably disposable, one-piece & close-fitting at ankles & wrists), gloves, hair covering & overshoes. ... clothing should be changed daily but ... discarded immediately if obvious contamination occurs ...

/also,/ workers should shower immediately. In chemical laboratory, gloves & gowns should always be worn ... however, gloves should not be assumed to provide full protection. Carefully fitted masks or respirators may be necessary when working with particulates or gases, & disposable plastic aprons might provide addnl protection. If gowns are of distinctive color, this is a reminder that they should not be worn outside of lab. /Chemical Carcinogens/

PRECAUTIONS FOR "CARCINOGENS": ... Operations connected with synth & purification ... should be carried out under well-ventilated hood. Analytical procedures ... should be carried out with care & vapors evolved during ... procedures should be removed. ... Expert advice should be obtained before existing fume cupboards are used ... & when new fume cupboards are installed. It is desirable that there be means for decreasing the rate of air extraction, so that carcinogenic powders can be handled without ... powder being blown around the hood. Glove boxes should be kept under negative air pressure. Air changes should be adequate, so that concn of vapors of volatile carcinogens will not occur. /Chemical Carcinogens/

PRECAUTIONS FOR "CARCINOGENS": Vertical laminar-flow biological safety cabinets may be used for containment of in vitro procedures ... provided that the exhaust air flow is sufficient to provide an inward air flow at the face opening of the cabinet, & contaminated air plenums that are under positive pressure are leak-tight. Horizontal laminar-flow hoods or safety cabinets, where filtered air is blown across the working area towards the operator, should never be used ... Each cabinet or fume cupboard to be used ... should be tested before work is begun (eg, with fume bomb) & label fixed to it, giving date of test & avg air-flow measured. This test should be repeated periodically & after any structural changes. /Chemical Carcinogens/

For more Preventive Measures (Complete) data for AMITROLE (18 total), please visit the HSDB record page.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

SMALL SPILLS AND LEAKAGE: If you spill this chemical, you should dampen the solid spill material with water, then transfer the dampened material to a suitable container. Use absorbent paper dampened with water to pick up any remaining material. Seal your contaminated clothing and the absorbent paper in a vapor-tight plastic bag for eventual disposal. Wash all contaminated surfaces 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 keep this material in a tightly closed container under an inert atmosphere, and store it at refrigerated temperatures. (NTP, 1992)

Store in an area without drain or sewer access. Separated from strong acids, strong oxidants, acid anhydrides and acid chlorides. Do NOT store or transport in containers made from iron, aluminium or copper and its alloys. Separated from food and feedstuffs.

Store at room temperature

PRECAUTIONS FOR "CARCINOGENS": Storage site should be as close as practical to lab in which carcinogens are to be used, so that only small quantities required for ... expt need to be carried. Carcinogens should be kept in only one section of cupboard, an explosion-proof refrigerator or freezer (depending on chemicophysical properties ...) that bears appropriate label. An inventory ... should be kept, showing quantity of carcinogen & date it was acquired ... . Facilities for dispensing ... should be contiguous to storage area. /Chemical Carcinogens/

Safe Storage of Pesticides. Always store pesticides in their original containers, complete with labels that list ingredients, directions for use, and first aid steps in case of accidental poisoning. Never store pesticides in cabinets with or near food, animal feed, or medical supplies. Do not store pesticides in places where flooding is possible or in places where they might spill or leak into wells, drains, ground water, or surface water.

7.2 Conditions for safe storage, including any incompatibilities

Store in an area without drain or sewer access. Separated from strong acids, strong oxidants, acid anhydrides and acid chlorides. Do NOT store or transport in containers made from iron, aluminium or copper and its alloys. Separated from food and feedstuffs.

Store at room temperature

PRECAUTIONS FOR "CARCINOGENS": Storage site should be as close as practical to lab in which carcinogens are to be used, so that only small quantities required for ... expt need to be carried. Carcinogens should be kept in only one section of cupboard, an explosion-proof refrigerator or freezer (depending on chemicophysical properties ...) that bears appropriate label. An inventory ... should be kept, showing quantity of carcinogen & date it was acquired ... . Facilities for dispensing ... should be contiguous to storage area. /Chemical Carcinogens/

Safe Storage of Pesticides. Always store pesticides in their original containers, complete with labels that list ingredients, directions for use, and first aid steps in case of accidental poisoning. Never store pesticides in cabinets with or near food, animal feed, or medical supplies. Do not store pesticides in places where flooding is possible or in places where they might spill or leak into wells, drains, ground water, or surface water.

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)

0.2 mg/m

(inhalable fraction): 0.2 mg/m

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: Amitrole appears as odorless white crystals or white powder. Bitter taste. Melting point 147-159 °C. Sublimes undecomposed at reduced pressure. Used as a post-emergence herbicide.

b) Odor: Odorless when pure.

c) Odor threshold: No data available

d) pH: FORMS NEUTRAL AQ SOLN BUT ACTS AS WEAK BASE WITH KB OF 1X10-10

e) Melting point/freezing point: 318 °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: 4.41e-07 mmHg at 68 °F (NTP, 1992)
l) Vapor density: No data available
m) Relative density: 1.138 at 68 °F (NTP, 1992) - Denser than water; will sink
n) Water solubility: greater than or equal to 100 mg/mL at 63.5 °F (NTP, 1992)
o) Partition coefficient: n-octanol/water: Log P (n-octanol/water): -0.4
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): 67.6 Å²
Complexity: 44

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

Light (decomposes), strong oxidizers [Note: Corrosive to iron, aluminum & copper].
Light (decomposes), strong oxidizers [Note: Corrosive to iron, aluminum & copper.]

10.6 Hazardous decomposition products

Thermal decomposition may produce: Carbon monoxide (CO), Carbon dioxide (CO□), Nitrogen oxides (NOx).
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:

Suspected of damaging fertility or the unborn child (H361).

Specific target organ toxicity (single exposure):

H372, H373

Specific target organ toxicity (repeated exposure):

No data available.

Aspiration hazard:

No data available.

11.2 Additional information

Carcinogen classification:

Amitrole

Group 3: Not classifiable as to its carcinogenicity to humans

Volume 79: (2001) Some Thyrotropic 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)

2001

2000

NB Overall evaluation downgraded to Group 3 with supporting evidence from other relevant data

Exposure routes:

The substance can be absorbed into the body by inhalation of its aerosol.

inhalation, ingestion, skin and/or eye contact

Signs and symptoms of exposure:

Redness.

Redness. Pain.

irritation eyes, skin; dyspnea (breathing difficulty), muscle spasms, ataxia, anorexia, salivation, increased body temperature; lassitude (weakness, exhaustion), skin dryness, depression (thyroid function suppression)

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

12. ECOLOGICAL INFORMATION

12.1 Toxicity

LC50 /Coturnix japonica/ (Japanese quail) oral >5000 ppm (no mortality to 5000 ppm), age 12 days.

LC50 /Phasianus colchicus/ (Ring-necked pheasant) >5000 ppm (no mortality to 5000 ppm), age 10 days.

LC50 Gammarus fasciatus (Scud) >10 mg/L/96 hr at 18 °C /static conditions without aeration/

LC50 /Pimephales promelas/ (Fathead minnow, weight 1.2 g) >100 mg/L/96 hr at 18 °C. /static conditions without aeration/

For more Ecotoxicity Values (Complete) data for AMITROLE (29 total), please visit the HSDB record page.

/BIRDS and MAMMALS/ Acute symptoms: ataxia, weakness, slight wing drop, during first 3 days after single oral admin only in /mallard ducks/.

/AQUATIC SPECIES/ /Investigators/ exposed fry of bluegill sunfish, green sunfish and lake chub sucker fish to amitrole at 50 mg/liter for 8 days and reported no deaths. Young bluegill survived a 12-day exposure to 25 mg/liter, although some deaths occurred at higher concentrations.

/AQUATIC SPECIES/ /Investigators/ exposed yearling Coho salmon (Oncorhynchus kisutch) to Amitrole-T at concentrations of between 0.25 and 200 mg/liter. Transfer of the young salmon to sea water with comparable concentrations of amitrole increased the toxic effect of the compound; 56% of fish survived 336 hr in sea water containing 25 mg amitrole/liter and 12.5% survived 50 mg/liter. According to the authors, deaths occurred within 24-48 hr. Smoltification, the adaptation of young salmon to sea water, is under thyroid control. The goitrogenic properties

12.2 Persistence and degradability

No data available.

12.3 Bioaccumulative potential

Log P (n-octanol/water): -0.4

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

This substance is classified as hazardous to the aquatic environment.

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)

Class 9

DOT label: Class 9

14.4 Packing group

Packing group III

14.5 Environmental hazards

Marine pollutant: Yes (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

Environmental 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 contains a chemical known to the State of California to cause cancer, birth defects, or other reproductive harm.

Other regulatory listings:

- The Australian Inventory of Industrial Chemicals: Chemical: 1H-1,2,4-Triazol-3-amine

- California Safe Cosmetics Program (CSCP) Reportable Ingredient: Hazard Traits - Carcinogenicity Authoritative List - NTP RoC - reasonable; Prop 65 Report - regardless of intended function of ingredient in the product

- EFSA Legal Basis: Commission Regulation (EU) No 1141/2010

- Status Regulation (EC): 01/21/EC, 2010/77/EU, Reg (EU) 2015/408, Reg. (EU) 2015/1885, Reg. (EU) 2016/871, Reg. (EU) No 540/2011

- 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.)

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: 2026/09/09

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.