Diatrizoic acid SDS/MSDS (Safety Data Sheet)

1. PRODUCT AND COMPANY IDENTIFICATION

Product identifier

* Product Name: Diatrizoic acid
* Catalog Number: S4563
* CAS Number: 117-96-4
* IUPAC Name: Benzoic acid, 3,5-bis(acetylamino)-2,4,6-triiodo-

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):

Skin sensitization: Category 1. H317

Respiratory sensitization: Category 1. H334

2.2 GHS Label elements, including precautionary statements

Hazard Pictogram(s)	
Signal Word	Danger
Hazard statement(s)	H317: May cause an allergic skin reaction H334: May cause allergy or asthma symptoms or breathing difficulties if inhaled
Precautionary statement(s)	None.
Prevention	P233: Keep container tightly closed. P260: Do not breathe dust/fume/gas/mist/vapors/spray. P261: Avoid breathing dust/fume/gas/mist/vapors/spray. P271: Use only outdoors or in a well-ventilated area. P272: Contaminated work clothing should not be allowed out of the workplace. P280: Wear protective gloves/protective clothing/eye protection/face protection/hearing protection. P284: [In case of inadequate ventilation] Wear respiratory protection.

Response	P302+P352: IF ON SKIN: wash with plenty of water. P304+P340: IF INHALED: Remove person to fresh air and keep comfortable for breathing. P321: Specific treatment (see information on this label and safety datasheet)). P333+P317: If skin irritation or rash occurs: Get medical help. P342+P316: If experiencing respiratory symptoms: Get emergence medical help immediately. P362+P364: Take off contaminated clothing and wash it before reuse.
Storage	P403: Store in a well-ventilated place.
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: Diatrizoic acid

CAS Number: 117-96-4

PubChem CID: 2140

Molecular formula: C11H9I3N2O4

Molecular weight: 613.91 g/mol

IUPAC name: 3,5-diacetamido-2,4,6-triiodobenzoic 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

Combustible. Heating may produce toxic fumes.

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

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.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Protect from light. Store at 20-25 °C (68-77 °F); avoid excessive heat.

7.2 Conditions for safe storage, including any incompatibilities

Protect from light. Store at 20-25 °C (68-77 °F); avoid excessive heat.

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 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

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: No data available

c) Odor threshold: No data available

d) pH: No data available

e) Melting point/freezing point: >250

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: VERY SLIGHTLY SOL IN WATER, ALCOHOL; SOL IN DIMETHYLFORMAMIDE, ALKALI HYDROXIDE SOLUTIONS

o) Partition coefficient: n-octanol/water: Log P (n-octanol/water): 1.8

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): 95.5 Å²

Complexity: 390

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 (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 allergy or asthma symptoms or breathing difficulties if inhaled (H334).

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

No additional toxicological information available.

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Diatrizoate's production and use as diagnostic contrast agent may result in its release to the environment through various waste streams. If released to air, an estimated vapor pressure of 3.6X10-15 mm Hg at 25 °C indicates diatrizoate will exist solely in the particulate phase in the atmosphere. Particulate-phase diatrizoate will be removed from the atmosphere by wet or dry deposition. Diatrizoate does not contain chromophores that absorb at wavelengths >290 nm and, therefore, is not expected to be susceptible to direct photolysis by sunlight. If released to soil, diatrizoate is expected to have very high mobility based upon an estimated Koc of 10. The estimated pKa of diatrizoate is 1.13, indicating that this compound will exist almost entirely in the anion form in the environment and anions generally do not adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts. Volatilization from moist soil is not expected because the compound exists as an anion and anions do not volatilize. Diatrizoate may not volatilize from dry soil surfaces based upon its estimated vapor pressure. Iodinated X-ray contrast agents are considered nondegradable by microorganisms. If released into water, diatrizoate is not expected to adsorb to suspended solids and sediment based upon the estimated Koc. The estimated pKa indicates diatrizoate will exist almost entirely in the anion form at pH values of 5 to 9 and, therefore, volatilization from water surfaces is n

12.2 Persistence and degradability

No data available.

12.3 Bioaccumulative potential

Log P (n-octanol/water): 1.8

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

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: Benzoic acid, 3,5-bis(acetylamino)-2,4,6-triiodo-

- FDA Requirements: The Approved Drug Products with Therapeutic Equivalence Evaluations List identifies currently marketed prescription drug products, incl diatrizoate meglumine, approved on the basis of safety and effectiveness by FDA under sections 505 of the Federal Food, Drug, and Cosmetic Act. /Diatrizoate meglum

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.