

## Chemical Safety Data Sheet MSDS / SDS

## 3,5-diacetamido-2,4,6-triiodobenzoic acid SDS

Revision Date:2024-04-25 Revision Number:1

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**SECTION 1: Identification of the substance/mixture and of the company/undertaking****Product identifier**

Product name: 3,5-diacetamido-2,4,6-triiodobenzoic acid

CAS: 117-96-4

**Relevant identified uses of the substance or mixture and uses advised against**

Relevant identified uses: For R&amp;D use only. Not for medicinal, household or other use.

Uses advised against: none

**Company Identification**

Company: Chemicalbook.in

Address: 5 vasavi Layout Basaveswara Nilayam Pragathi Nagar Hyderabad, India -500090

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**SECTION 2: Hazards identification****Classification of the substance or mixture**

Not classified.

**GHS label elements, including precautionary statements**

Signal word                      No signal word

**Hazard statement(s)**

none

**Precautionary statement(s)****Prevention**

none

**Response**

none

**Storage**

none

**Disposal**

none

**Other hazards which do not result in classification**

no data available

**SECTION 3: Composition/information on ingredients****Substance**

Chemical name:                      3,5-diacetamido-2,4,6-triiodobenzoic acid

Common names and  
synonyms:                      3,5-diacetamido-2,4,6-triiodobenzoic acid

CAS number:                      117-96-4

EC number:                      204-223-6

Concentration:                      100%

## SECTION 4: First aid measures

### Description of necessary first-aid measures

#### If inhaled

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately. Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

#### Following skin contact

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

#### Following eye contact

Rinse with pure water for at least 15 minutes. Consult a doctor.

#### Following ingestion

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison Control Center immediately.

### Most important symptoms/effects, acute and delayed

no data available

### Indication of immediate medical attention and special treatment needed, if necessary

For major life-threatening reactions, careful monitoring of vital signs and emergency therapy, including artificial respiration with oxygen, if needed for respiratory depression, and cardiac massage in the event of cardiac arrest. To restore blood pressure, administration of intravenous fluids and/or vasopressors. If hypotension requires the use of vasopressors, slow infusion of ... norepinephrine or ... phenylephrine, appropriately diluted. If hypotension is due to increased vagal activity (vasovagal reaction), intravenous administration of atropine, repeated in one to two hours if needed. Other specific treatment may include: Epinephrine for acute allergic-like or anaphylactoid reactions; Diphenhydramine for minor allergic-like reactions; diazepam or phenobarbital to control convulsions ...

## SECTION 5: Firefighting measures

### Suitable extinguishing media

Use dry chemical, carbon dioxide or alcohol-resistant foam.

**Specific hazards arising from the chemical**

no data available

**Special protective actions for fire-fighters**

Wear self-contained breathing apparatus for firefighting if necessary.

**SECTION 6: Accidental release measures****Personal precautions, protective equipment and emergency procedures**

Avoid dust formation. Avoid breathing mist, gas or vapours. Avoid contacting with skin and eye. Use personal protective equipment. Wear chemical impermeable gloves. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

**Environmental precautions**

Prevent further spillage or leakage if it is safe to do so. Do not let the chemical enter drains. Discharge into the environment must be avoided.

**Methods and materials for containment and cleaning up**

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

**SECTION 7: Handling and storage****Precautions for safe handling**

Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

**Conditions for safe storage, including any incompatibilities**

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

## SECTION 8: Exposure controls/personal protection

### Control parameters

### Occupational Exposure limit values

no data available

### Biological limit values

no data available

### Appropriate engineering controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

### Individual protection measures, such as personal protective equipment (PPE)

#### Eye/face protection

Wear tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

#### Skin protection

Wear fire/flame resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

#### Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

#### Thermal hazards

no data available

## SECTION 9: Physical and chemical properties and safety characteristics

Physical state: Solid

Colour: WHITE POWDER

Odour: no data available

Melting point/freezing point:	>300°C
Boiling point or initial boiling point and boiling range:	614.1°C at 760 mmHg
Flammability:	no data available
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	325.2°C
Auto-ignition temperature:	no data available
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	no data available
Solubility:	VERY SLIGHTLY SOL IN WATER, ALCOHOL; SOL IN DIMETHYLFORMAMIDE, ALKALI HYDROXIDE SOLUTIONS
Partition coefficient n-octanol/water:	no data available
Vapour pressure:	6.19E-16mmHg at 25°C
Density and/or relative density:	2.619 g/cm <sup>3</sup>
Relative vapour density:	no data available
Particle characteristics:	no data available

## SECTION 10: Stability and reactivity

### Reactivity

no data available

### Chemical stability

Preparations containing diatrizoate sodium should be protected from strong light.

### Possibility of hazardous reactions

no data available

### Conditions to avoid

no data available

### Incompatible materials

no data available

### Hazardous decomposition products

When heated to decomposition it emits very toxic fumes of /oxides of nitrogen and iodine/.

## SECTION 11: Toxicological information

### Acute toxicity

Oral: no data available

Inhalation: no data available

Dermal: no data available

### Skin corrosion/irritation

no data available

### Serious eye damage/irritation

no data available

**Respiratory or skin sensitization**

no data available

**Germ cell mutagenicity**

no data available

**Carcinogenicity**

no data available

**Reproductive toxicity**

no data available

**STOT-single exposure**

no data available

**STOT-repeated exposure**

no data available

**Aspiration hazard**

no data available

**SECTION 12: Ecological information**

**Toxicity**

Toxicity to fish: no data available

Toxicity to daphnia and other aquatic invertebrates: no data available

Toxicity to algae: no data available

Toxicity to microorganisms: no data available



### Persistence and degradability

AEROBIC: Iodinated X-ray contrast agents are considered nondegradable by microorganisms(1,2). However when incubated with 1mM diatrizoate at 30 deg C for 32 days, the fungus *Trametes versicolor*, has been shown to partially diiodinate C-14 ring-labeled diatrizoate, liberating traces of  $^{14}\text{CO}_2$ (1). The three main metabolites identified were 3,5-di(acetamido)-2,6-diiodobenzoic acid, 3,5-di(acetamido)-2,4-diiodobenzoic acid, and 3,5-di(acetamido)-2-iodobenzoic acid(1).[(1) Rode U, Muller R; *Appl Environ Microbiol* 64: 3114-7 (1998) (2) Perez S et al; pp. 113-44 in *Topical Issues in Applied Microbiology and Biotechnology*. Kerala, India: Research Signpost (2006)] Full text: PMC106829

### Bioaccumulative potential

An estimated BCF of 3 was calculated in fish for diatrizoate(SRC), using an estimated log Kow of 1.37(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

### Mobility in soil

Using a structure estimation method based on molecular connectivity indices(1), the Koc of diatrizoate can be estimated to be 10(SRC). According to a classification scheme(2), this estimated Koc value suggests that diatrizoate is expected to have very high mobility in soil. Iodinated diagnostic contrast agents such as diatrizoate leach readily into groundwater(3). The estimated pKa of diatrizoate is 1.13(4), 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(5).

### Other adverse effects

no data available

## SECTION 13: Disposal considerations

### Disposal methods

#### Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

#### Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas

scrubbing is possible for combustible packaging materials.

## SECTION 14: Transport information

### UN Number

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

### UN Proper Shipping Name

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

### Transport hazard class(es)

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

### Packing group, if applicable

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

### Environmental hazards

ADR/RID: No

IMDG: No

IATA: No

### Special precautions for user

no data available

### Transport in bulk according to IMO instruments

no data available

## SECTION 15: Regulatory information

Safety, health and environmental regulations specific for the product in question

European Inventory of Existing Commercial Chemical Substances (EINECS)

Listed.

EC Inventory

Listed.

United States Toxic Substances Control Act (TSCA) Inventory

Not Listed.

China Catalog of Hazardous chemicals 2015

Not Listed.

New Zealand Inventory of Chemicals (NZIoC)

Not Listed.

(PICCS)

Not Listed.

Vietnam National Chemical Inventory

Not Listed.

IECSC)

Not Listed.

Korea Existing Chemicals List (KECL)

Not Listed.

## SECTION 16: Other information

### **Abbreviations and acronyms**

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

### **References**

IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>

HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:  
[http://www.echemportal.org/echemportal/index?pageID=0&request\\_locale=en](http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en)

CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

ERG - Emergency Response Guidebook by U.S. Department of Transportation, website:  
<http://www.phmsa.dot.gov/hazmat/library/erg>

Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

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