

## Chemical Safety Data Sheet MSDS / SDS

## N-[4-[[[(2,4-diamino-6-pteridiny)l)methyl]methylamino]benzoyl]-DL-glutamic 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: N-[4-[[[(2,4-diamino-6-pteridiny)l)methyl]methylamino]benzoyl]-DL-glutamic acid

CAS: 60388-53-6

**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**

no data available

**GHS label elements, including precautionary statements**

Signal word                   no data available

**Hazard statement(s)**

no data available

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

no data available

**Response**

no data available

**Storage**

no data available

**Disposal**

no data available

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

no data available

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

Chemical name:               N-[4-[[[(2,4-diamino-6-pteridiny)l)methyl]methylamino]benzoyl]-DL-glutamic acid

Common names and  
synonyms:                   N-[4-[[[(2,4-diamino-6-pteridiny)l)methyl]methylamino]benzoyl]-DL-glutamic acid

CAS number:                 60388-53-6

EC number:                 262-213-7

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

Leucovorin is indicated to diminish the toxicity and counteract the effect of inadvertently administered overdoses of methotrexate. Leucovorin administration should begin as promptly as possible. As the time interval between methotrexate administration and leucovorin initiation increases, the effectiveness of leucovorin in counteracting toxicity decreases. Monitoring of the serum methotrexate concentration is essential in determining the optimal dose and duration of treatment with leucovorin.

## 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**

Methotrexate sodium tablets should be protected from light and stored in well-closed containers at 15-30 deg C. Methotrexate sodium injection and powder for injection should be protected from light and stored at 15-30 deg C. Methotrexate sodium

## **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: yellow to orange crystalline powder

Colour: Orange-brown, crystalline powder

Odour: no data available

Melting point/freezing point:	195°C (dec.)(lit.)
Boiling point or initial boiling point and boiling range:	no data available
Flammability:	no data available
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	no data available
Auto-ignition temperature:	no data available
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	no data available
Solubility:	Insoluble in water , alcohol, chloroform, ether; slightly soluble in dilute hydrochloric acid; soluble in dil solns of alkali hydroxides and carbonates.
Partition coefficient n-octanol/water:	log Kow = -1.85
Vapour pressure:	2.1X10 <sup>-19</sup> mm Hg at 25 deg C /Estimated/
Density and/or relative density:	1.536 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

no data available

### 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 toxic fumes including /nitrogen oxides/.

## SECTION 11: Toxicological information

### Acute toxicity

Oral: LD50 Rat oral 180 +/- 45 mg/kg body weight

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**

Classification of carcinogenicity: 1) evidence in humans: Inadequate data; 2) evidence in animals: Inadequate data. Overall summary evaluation of carcinogenic risk to humans is Group 3: The agent is not classifiable as to its carcinogenicity to humans. From table

#### **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: An OECD confirmatory test was carried out in a laboratory-scale treatment plant, using a sludge inoculum from the municipal sewage plant in Bochum-Olbachtal, Germany(1). The test was run for 10 days, flow rate of 1 L/hr, and a retention time of 3 hrs. Methotrexate, at concentrations of 10 and 20 mg/L, at both concns, the compound reached a rate of 95% biodegradation after approximately 8 days, with a maximum rate of 98% biodegradation measured at 10 days; however, the biodegradation process resulted in the formation of 7-hydroxymethotrexate which is toxic and persistent(1). When presented as a mixture including cyclophosphamide (150 mg/L), cytarabine (12.5 mg/L), and 5-fluorouracil (5.0 mg/L), methotrexate (4.0 mg/L) exhibited a similar biodegradation rate(1).

### **Bioaccumulative potential**

An estimated BCF of 3.2 was calculated for methotrexate(SRC), using a log Kow of -1.85(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), provided the compound is not altered physically or chemically once released into the environment(SRP).

### **Mobility in soil**

The Koc of methotrexate is estimated as 1(SRC), using a log Kow of -1.85(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that methotrexate is expected to have very high mobility in soil. The pKa of the carboxylic acid moiety of methotrexate is 4.70(4), indicating that this compound will primarily exist in anion form in the environment and anions generally do not adsorb more strongly to organic carbon and clay than their neutral counterparts(5). However, aromatic amines are expected to bind strongly to humus or organic matter in soils due to the high reactivity of the aromatic amino group(6,7), suggesting that mobility may be much lower in some soils(SRC).

### **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: UN1544 (For reference only, please check.)

IMDG: UN1544 (For reference only, please check.)

IATA: UN1544 (For reference only, please check.)

### **UN Proper Shipping Name**

ADR/RID: ALKALOIDS, SOLID, N.O.S. or ALKALOID SALTS, SOLID, N.O.S. (For reference only, please check.)

IMDG: ALKALOIDS, SOLID, N.O.S. or ALKALOID SALTS, SOLID, N.O.S. (For reference only, please check.)

IATA: ALKALOIDS, SOLID, N.O.S. or ALKALOID SALTS, SOLID, N.O.S. (For reference only, please check.)

### **Transport hazard class(es)**

ADR/RID: 6.1 (For reference only, please check.)

IMDG: 6.1 (For reference only, please check.)

IATA: 6.1 (For reference only, please check.)

### **Packing group, if applicable**

ADR/RID: I (For reference only, please check.)

IMDG: I (For reference only, please check.)

IATA: I (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/>

properties of the product. We as supplier shall not be held liable for any