ChemicalBook

Chemical Safety Data Sheet MSDS / SDS

(+/-)AMETHOPTERIN

Revision Date:2024-11-02 Revision Number:1

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

Product identifier

Product name	: (+/-)AMETHOPTERIN
CBnumber	: CB7749012
CAS	: 60388-53-6
EINECS Number	: 262-213-7
Synonyms	: DL-Amethopterin,Methotrexate Impurity 3

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

Relevant identified uses	: For R&D use only. Not for medicinal, household or other use.
Uses advised against	: none

Company Identification

Company	: Chemicalbook
Address	: Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone	: 010-86108875

SECTION 2: Hazards identification

Classification of the substance or mixture

no data available

Label elements

Pictogram(s)

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

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no data available

Other hazards

no data available

SECTION 3: Composition/information on ingredients

Substance

Product name	: (+/-)AMETHOPTERIN
Synonyms	: DL-Amethopterin,Methotrexate Impurity 3
CAS	: 60388-53-6
EC number	: 262-213-7
MF	: C20H22N8O5
MW	: 454.44

SECTION 4: First aid measures

Description of 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 and effects, both acute and delayed

no data available

Indication of any immediate medical attention and special treatment needed

Leucovorin is indicated to diminish the toxicity and counteract the effect of inadvertently administered overdosages 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

Extinguishing media

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

Specific Hazards Arising from the Chemical

no data available

Advice for firefighters

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

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SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

no data available

Biological limit values

no data available

Exposure 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

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

Information on basic physicochemical properties

Physical state	powder
Colour	yellow
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	H_2O: Add a minimal amount of 0.1燦 NaOH to solubilize, then dilute in neutral buffer or saline. Diluted stock is stable for 1爓eek refrigerated and for 1爓onth frozen at?#8722;20?#x00b0;C.insoluble
Partition coefficient n-octanol/water	log Kow = -1.85
Vapour pressure	2.1X10-19 mm Hg at 25 deg C /Estimated/
Density and/or relative density	1.536 g/cm3
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

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/