

Chemical Safety Data Sheet MSDS / SDS

2,6-DIMETHYLANILINE HYDROCHLORIDERevision Date:2024-07-20 Revision Number:1

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

Product name : 2,6-DIMETHYLANILINE HYDROCHLORIDE
CBnumber : CB6299479
CAS : 21436-98-6
EINECS Number : 244-388-1
Synonyms : Ropivacaine related compound A,2,6-Dimethylaniline Hydrochloride

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 : 400-158-6606

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

no data available

Other hazards

no data available

SECTION 3: Composition/information on ingredients

Substance

Product name	: 2,6-DIMETHYLANILINE HYDROCHLORIDE
Synonyms	: Ropivacaine related compound A,2,6-Dimethylaniline Hydrochloride
CAS	: 21436-98-6
EC number	: 244-388-1
MF	: C ₈ H ₁₂ ClN
MW	: 157.64

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

Immediate First Aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand-valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR if necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. Aromatic hydrocarbons and related compounds

SECTION 5: Firefighting measures

Extinguishing media

Suitable extinguishing media: Use water spray, alcohol-resistant foam, dry chemical, or carbon dioxide.

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

ACCIDENTAL RELEASE MEASURES: Personal precautions, protective equipment and emergency procedures: Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapors accumulating to form explosive concentrations. Vapors can accumulate in low areas. Environmental precautions: Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided. Methods and materials for containment and cleaning up: Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations. Keep in suitable, closed containers for disposal.

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

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

Component	2,6-xylidinium chloride
CAS No.	21436-98-6
	Recommended Exposure Limit: 10-hour Time-Weighted Average: 2 ppm (10 mg/cu m). Skin.

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/flamm 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 or crystals
Colour	White to Pale Brown
Odour	Characteristic odor
Melting point/freezing point	188°C(lit.)
Boiling point or initial boiling point and boiling range	131°C/2.5mmHg(lit.)
Flammability	no data available
Lower and upper explosion limit/flammability limit	no data available
Flash point	57°C(lit.)
Auto-ignition temperature	520 deg C
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	1.7 mPa.s (dynamic) at 50 deg C
Solubility	DMSO (Slightly), Methanol (Slightly, Sonicated)
Partition coefficient n-octanol/water	log Kow = 1.84
Vapour pressure	0.13mmHg at 25°C
Density and/or relative density	0.9842 g/cu cm at 20 deg C
Relative vapour density	4.2 (Air = 1)

SECTION 10: Stability and reactivity

Reactivity

no data available

Chemical stability

Stable under recommended storage conditions.

Possibility of hazardous reactions

This chemical is a combustible liquid. Xylidines

Conditions to avoid

no data available

Incompatible materials

Incompatible materials: Acids, acid chlorides, acid anhydrides, oxidizing agents, chloroformates, halogens.

Hazardous decomposition products

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

SECTION 11: Toxicological information

Acute toxicity

- Oral: LD50 Rat oral 840 mg/kg
- 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

Evaluation: There is inadequate evidence in humans for the carcinogenicity of 2,6-dimethylaniline. There is sufficient evidence in experimental

animals for the carcinogenicity of 2,6-dimethylaniline. Overall evaluation: 2,6-dimethylaniline is possibly carcinogenic to humans (Group 2B).

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: A Warburg respirometer study utilizing an activated sludge seed and 6 hr of incubation resulted in a 2,6-xylydine depletion of 33-37% at a concentration of 20 ppm(1). In a 6 week soil degradation study using (14)C-labelled 2,6-xylydine, 8.4% of applied radioactivity was recovered via CO₂ evolution in non-autoclaved soil while 0% CO₂ evolution occurred in autoclaved soil(2). In a soil degradation study conducted in glass vessels using Chernozem soil, 2,6-xylydine (at 500 mg/L) was degraded after 3 days of incubation with >90% recovered in transformation products(3). Using OECD Guideline 301F (Ready Biodegradability: Manometric Respirometry Test), 2,6-xylydine (at 100 mg/L) reached 4, 8, 25, 38 and 69% of its theoretical BOD after 7, 13, 36, 42 and 70 days. respectively(4); these results indicated that 2,6-xylydine was not readily biodegradable according to OECD criteria, however, it is biodegradable after extended adaptation(4). In another OECD Guideline 301F study, 2,6-xylydine (at 100 mg/L) showed no biodegradation after 33 day(4). Using OECD Guideline 302B (Inherent biodegradability: Zahn-Wellens/EMPA Test) and an industrial activated sludge seed, 83% of initial 2,6-xylydine was removed from the aqueous test system after 11 days, however, the substance was mainly removed via volatilization(4). 2,6-Xylydine, present at 100 mg/L, reached 0% of its theoretical BOD in 4 weeks using an activated sludge inoculum at 30 mg/L in the Japanese MITI test(5).

Bioaccumulative potential

An estimated BCF value of 8 was calculated for 2,6-xylydine in fish(SRC), using a log K_{ow} of 1.84(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF value suggests that bioconcentration in aquatic organisms is low(SRC).

Mobility in soil

Using a structure estimation method based on molecular connectivity indices(1), the K_{oc} of 2,6-xylydine can be estimated to be 190(SRC). According to a classification scheme(2), this estimated K_{oc} value suggests that 2,6-xylydine is expected to have moderate mobility in soil. Aromatic amines are expected to bind strongly to humus or organic matter in soils due to the high reactivity of the aromatic amino group(3,4), suggesting that mobility may be lower in some soils(SRC). In a short term soil adsorption study using 14C-labelled 2,6-xylydine, 66% of the

applied radioactivity was bound to the soil (3.4% organic matter, 36.6% sand, 28.2% silt, 35.2% clay) after 24 hrs(3).

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: UN3272 (For reference only, please check.)

IMDG: UN3272 (For reference only, please check.)

IATA: UN3272 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: ESTERS, N.O.S. (For reference only, please check.)

IMDG: ESTERS, N.O.S. (For reference only, please check.)

IATA: ESTERS, N.O.S. (For reference only, please check.)

Transport hazard class(es)

ADR/RID: 3 (For reference only, please check.)

IMDG: 3 (For reference only, please check.)

IATA: 3 (For reference only, please check.)

Packing group, if applicable

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

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

IATA: II (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?pagelD=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/>

Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.