

Chemical Safety Data Sheet MSDS / SDS

Citalopram-D6 HBr

Revision Date:2026-05-31 Revision Number:1

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

Product identifier

Product name : Citalopram-D6 HBr
CBnumber : CB72558898
CAS : 1190003-26-9
EINECS Number : 200-659-6
Synonyms : Citalopram-D6 HBr

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

GHS Label elements, including precautionary statements

Symbol(GHS)



Signal word

Danger

Precautionary statements

P311 Call a POISON CENTER or doctor/physician.
P301+P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.
P280 Wear protective gloves/protective clothing/eye protection/face protection.
P260 Do not breathe dust/fume/gas/mist/vapours/spray.
P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.

Hazard statements

H370 Causes damage to organs
H225 Highly Flammable liquid and vapour

SECTION 3: Composition/information on ingredients

Substance

Product name	: Citalopram-D6 HBr
Synonyms	: Citalopram-D6 HBr
CAS	: 1190003-26-9
EC number	: 200-659-6
MF	: C ₂₀ H ₂₁ N ₂ O
MW	: 324.4

SECTION 4: First aid measures

General advice

First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Call a physician immediately.

In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

If swallowed

After swallowing: fresh air. Make victim drink ethanol (e.g. 1 drinking glass of a 40% alcoholic beverage). Call a doctor immediately (mention methanol ingestion). Only in exceptional cases, if no medical care is available within one hour, induce vomiting (only in fully conscious persons) and make victim drink ethanol again (approx. 0.3 ml of a 40% alcoholic beverage/kg body weight/hour).

Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2) and/or in section 11

Protection of first-aiders

For personal protection see section 8.

Notes to physician

No data available

SECTION 5: Firefighting measures

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

Specific hazards during fire fighting

Pay attention to flashback. Vapors are heavier than air and may spread along floors. Forms explosive mixtures with air at ambient temperatures.

Specific extinguishing methods

Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.

Special protective equipment for fire-fighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert. Advice for emergency responders: For personal protection see section 8.

Environmental precautions

Do not let product enter drains. Risk of explosion.

Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully with liquid-absorbent material. Dispose of properly. Clean up affected area.

SECTION 7: Handling and storage

Handling

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Advice on safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Avoidance of contact

Acids Oxidizing agents Alkali metals Strong oxidizing agents Strong acids Acid chlorides Acid anhydrides Reducing agents Strong reducing agents Phosphorus halides

Storage

Further information on storage conditions

Keep container tightly closed in a dry and wellventilated place. Keep away from heat and sources of ignition. Keep locked up or in an area accessible only to qualified or authorized persons.

Storage class

3, Flammable liquids

Recommended storage temperature

-20 °C

SECTION 8: Exposure controls/personal protection

Ingredients with workplace control parameters

Biological occupational exposure limits soon as possible after exposure ceases)

Engineering measures

No data available

Personal protective equipment**Respiratory protection**

required when vapours/aerosols are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter type

Filter type ABEK

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Safety glasses

Skin and body protection

Flame retardant antistatic protective clothing.

Hand protection**Material**

butyl-rubber

Break through time

480 min

Glove thickness

0.3 mm

Protective index

Full contact

Manufacturer

Butoject® (KCL 897 / Aldrich Z677647, Size M)

Material

Nitrile rubber

Break through time

30 min

Glove thickness

0.4 mm

Protective index

Splash contact

Manufacturer

Camatril® (KCL 730 / Aldrich Z677442, Size M)

Manufacturer

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

Remarks

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it. If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

liquid

Color

Colourless to Light Yellow

Odor

No data available

Odor Threshold

No data available

pH

No data available

Melting point/ range

No data available

Boiling point/boiling range

64 - 65 °C (1.013 hPa) Flash point: 9.7 °C

Method: closed cup

Evaporation rate

No data available

Flammability (solid, gas)

No data available

Flammability (liquids)

No data available

Burning rate

No data available

Upper explosion limit / Upper flammability limit

36 %(V)

Lower explosion limit / Lower flammability limit

6 %(V)

Vapor pressure

No data available

Relative vapor density

No data available

Relative density

No data available

Density

0.791 g/cm³ (20 °C)

Water solubility

No data available

Partition coefficient: n-octanol/water

No data available

Autoignition temperature

No data available

Decomposition temperature

No data available

Viscosity, dynamic

No data available

Viscosity, kinematic

No data available

Flow time

No data available

Explosive properties

Not classified as explosive.

Oxidizing properties

none

Particle characteristics Particle size

No data available

Flash point

9°C

Solubility

Acetonitrile (Slightly), Aqueous Acid (Slightly), Chloroform (Slightly)

Physical state

Thick Oil to Solid

SECTION 10: Stability and reactivity

Reactivity

Vapors may form explosive mixture with air.

Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

Possibility of hazardous reactions

No data available

Conditions to avoid

Warming.

Incompatible materials

Acids Oxidizing agents Alkali metals Strong oxidizing agents Strong acids Acid chlorides Acid anhydrides Reducing agents Strong reducing agents Phosphorus halides

Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects**Mixture Acute toxicity**

Oral: No data available

Acute toxicity estimate Inhalation - 4 h - 3.1 mg/l - vapor (Calculation method)

Acute toxicity estimate Dermal - 300.13 mg/kg (Calculation method)

Skin corrosion/irritation

Classified based on available data. For more details, see section 2

Serious eye damage/eye irritation

Classified based on available data. For more details, see section 2

Respiratory or skin sensitization

Classified based on available data. For more details, see section 2

Germ cell mutagenicity

Classified based on available data. For more details, see section 2

Carcinogenicity

Classified based on available data. For more details, see section 2

Reproductive toxicity

Classified based on available data. For more details, see section 2

Specific target organ toxicity - single exposure

Mixture causes damage to organs. - Eyes

Specific target organ toxicity - repeated exposure

Classified based on available data. For more details, see section 2

Aspiration hazard

Classified based on available data. For more details, see section 2

11.2 Additional Information

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Methyl alcohol may be fatal or cause blindness if swallowed., Cannot be made non- poisonous., Effects due to ingestion may include:, Nausea, Headache, Vomiting,

Gastrointestinal disturbance, Dizziness, Weakness, Confusion.

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

Components Methanol

Acute toxicity

Acute toxicity estimate Oral - 100.1 mg/kg (Expert judgment)

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Symptoms: Nausea, Vomiting

Acute toxicity estimate Inhalation - 4 h - 3.1 mg/l - vapor (Expert judgment)

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Symptoms: Irritation symptoms in the respiratory tract.

Acute toxicity estimate Dermal - 300.1 mg/kg (Expert judgment)

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation

Remarks: (ECHA)

Remarks: Drying-out effect resulting in rough and chapped skin.

Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation

Remarks: (ECHA)

Respiratory or skin sensitization

Sensitisation test: - Guinea pig

Result: negative (OECD Test Guideline 406)

Germ cell mutagenicity

Based on available data the classification criteria are not met.

Test Type: Ames test

Test system: Salmonella typhimurium

Result: negative

Test Type: In vitro mammalian cell gene mutation test

Test system: Chinese hamster lung cells

Result: negative

Method: OECD Test Guideline 474

Species: Mouse - male and female - Bone marrow

Result: negative

Carcinogenicity

Did not show carcinogenic effects in animal experiments.

Reproductive toxicity

Based on available data the classification criteria are not met.

Specific target organ toxicity - single exposure

Causes damage to organs. - Eyes, Central nervous system

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Acute oral toxicity - Nausea, Vomiting

Acute inhalation toxicity - Irritation symptoms in the respiratory tract.

Specific target organ toxicity - repeated exposure

Classified based on available data. For more details, see section 2

Aspiration hazard

Classified based on available data. For more details, see section 2

SECTION 12: Ecological information

Ecotoxicity

Components:

Methanol:

Toxicity to fish

LC50 (Lepomis macrochirus (Bluegill)): 15,400.0 mg/l End point: mortality Exposure time: 96 h Test Type: flow-through test Analytical monitoring: yes Method: US-EPA

Toxicity to daphnia and other aquatic invertebrates

EC50 (*Daphnia magna* (Water flea)): 18,260 mg/l End point: Immobilization Exposure time: 96 h Test Type: semi-static test Method: OECD Test Guideline 202

Toxicity to algae/aquatic plants

ErC50 (*Pseudokirchneriella subcapitata* (green algae)): ca. 22,000.0 mg/l Exposure time: 96 h Test Type: static test Method: OECD Test Guideline 201

Toxicity to fish (Chronic toxicity)

NOEC (*Oryzias latipes* (Orange-red killifish)): 7,900 mg/l Exposure time: 200 h Remarks: (External MSDS)

Toxicity to microorganisms

IC50 (activated sludge): > 1,000 mg/l Exposure time: 3 h Test Type: static test Analytical monitoring: yes Method: OECD Test Guideline 209

Persistence and degradability

Components:

Methanol:

Biodegradability

Result: Readily biodegradable. Biodegradation: 99 % Exposure time: 30 d Method: OECD Test Guideline 301D

Biochemical Oxygen Demand (BOD)

600 - 1,120 mg/g Incubation time: 5 d Remarks: (IUCLID)

Chemical Oxygen Demand (COD)

1,420 mg/g Remarks: (IUCLID)

ThOD

1,500 mg/g Remarks: (Lit.)

BOD/ThOD

76 % Remarks: Closed Bottle test (IUCLID)

Stability in water

Hydrolysis: 83 - 91 % at 19 °C(72 h) Remarks: Hydrolyzes on contact with water. Hydrolyzes readily. Degradation half life: 2.2 yr Remarks: reaction with hydroxyl radicals (IUCLID)

Photodegradation

Degradation (direct photolysis): 50 % Degradation half life: 17.2 d

Bioaccumulative potential

Components:

Methanol:

Bioaccumulation

Species: *Cyprinus carpio* (Carp) Bioconcentration factor (BCF): 1.0 Exposure time: 72 d Temperature: 20 °C Concentration: 5 mg/l

Partition coefficient: noctanol/water

log Pow: -0.77 (25 °C) Method: (experimental) Remarks: (HSDB) Bioaccumulation is not expected.

Mobility in soil

Components:

Methanol:

Stability in soil

Remarks: Will not adsorb on soil.

Other adverse effects**Components:****Methanol:****Results of PBT and vPvB assessment**

Substance is not persistent, bioaccumulative, and toxic (PBT).

Additional ecological information

Avoid release to the environment.

SECTION 13: Disposal considerations

Disposal methods**Waste from residues**

Offer surplus and non-recyclable solutions to a licensed disposal company.

SECTION 14: Transport information

International Regulations**IATA-DGR**

UN/ID No. : UN 1230

Proper shipping name : Methanol solution

Class : 3

Subsidiary risk : 6.1

Packing group : II

Labels : Class 3 - Flammable liquids, Division 6.1 - Toxic substances

Packing instruction (cargo aircraft) : 364

Packing instruction (passenger aircraft) : 352

IMDG-Code

UN number : UN 1230

Proper shipping name : METHANOL SOLUTION

Class : 3

Subsidiary risk : 6.1

Packing group : II

Labels : 3 (6.1)

EmS Code : F-E, S-D

Marine pollutant : no

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable for product as supplied.

National regulation GB 6944/12268

UN number : UN 1230

Proper shipping name : METHANOL

Class : 3

Subsidiary risk : 6.1

Packing group : II

Labels : 3 (6.1)

Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

SECTION 15: Regulatory information

National regulatory information

Law on the Prevention and Control of Occupational Diseases

Regulations on Safety Management of Hazardous Chemicals

Identification of Major Hazard Installations for Hazardous Chemicals (GB 18218)

No. / Code Chemical name / Category Threshold quantity

W5.3 Flammable liquids 1,000 t

Catalogue of Specially Controlled Hazardous

Listed Chemicals

List of Explosive Precursors

Not listed

Regulation on the Administration of Precursor Chemicals

Catalogue and Classification of Precursor Chemicals

Not listed

Regulations on the Administration of Controlled Chemicals

List of Controlled Chemicals

Not listed

Regulations of Ozone Depleting Substances Management

List of Controlled Ozone Depleting Substances

Not listed

List of Controlled Ozone Depleting Substances Import and Export

Not listed

Environmental Protection Law

List of Priority Controlled Chemicals

Not listed

List of Key Controlled New Pollutants

Not listed

SECTION 16: Other information

Full text of other abbreviations

ACGIH

USA. ACGIH Threshold Limit Values (TLV)

ACGIH BEI

ACGIH - Biological Exposure Indices (BEI)

GBZ 2.1-2007

Occupational exposure limits for hazardous agents in the workplace - Chemical hazardous agents.

ACGIH / TWA

8-hour, time-weighted average

ACGIH / STEL

Short-term exposure limit

GBZ 2.1-2007 / PC-TWA

Permissible concentration - time weighted average

GBZ 2.1-2007 / PC-STEL AIC - Australian Invent Transport by Land of Bra bw - Body weight; CMR Standard of the German List (Canada); ECx - Conc associated with x%respo Chemical Substances (Jap response; ERG - Emerge GLP - Good Laboratory P cer; IATA - International Construction and Equipm Half maximal inhibitory c tion; IECSC - Inventory o tional Maritime Dangerou Industrial Safety and H Standardization; KECI - K tration to 50 %of a test (Median Lethal Dose); MA lution from Ships; n.o.s. No Observed (Adverse) E fect Level; NOELR - No Norm; NTP - National Toxi icals; OECD - Organizatio fice of Chemical Safety a and Toxic substance; PIC stances; (Q)SAR - (Quant (EC) No 1907/2006 of th Registration, Evaluation, Accelerating Decompositi Chemical Substance Inve Thailand Existing Chemicala States); UN - United Nat Transport of Dangerous WHMIS - Workplace Hazar

Permissible concentration - short term exposure limit ry of Industrial Chemicals

ANTT - National Agency for il

ASTM - American Society for the Testing of Materials

- Carcinogen, Mutagen or Reproductive Toxicant

DIN nstitute for Standardisation

DSL - Domestic Substances notification associated with x% response

ELx - Loading rate

EmS - Emergency Schedule

ENCS - Existing and New n)

ErCx - Concentration associated with x% growth rate

cy Response Guide

GHS - Globally Harmonized System

actice

IARC - International Agency for Research on Cancer

IBC - International Code for the construction of Ships carrying Dangerous Chemicals in Bulk

IC50 concentration

ICAO - International Civil Aviation Organization- Existing Chemical Substances in China

IMDG - International Goods

IMO - International Maritime Organization

ISHL - Health Law (Japan)

ISO - International Organisation for Standardization Existing Chemicals Inventory

LC50 - Lethal Concentration

LD50 - Lethal Dose to 50% of a test population

POL - International Convention for the Prevention of Pollution from Ships - Not Otherwise Specified

NCh - Chilean Norm

NO(A)EC - No Effect Concentration

NO(A)EL - No Observed (Adverse) Effect Loading Rate

NOM - Official Mexican Nomenclature Program

NZIoC - New Zealand Inventory of Chemicals for Economic Co-operation and Development

OPPTS - Office of Pollution Prevention

PBT - Persistent, Bioaccumulative and Toxic - Philippines Inventory of Chemicals and Chemical Substances) Structure Activity Relationship

REACH - Regulation of the European Parliament and of the Council concerning the restriction and restriction of Chemicals

SADT - Self-heating Temperature

SDS - Safety Data Sheet

TCSI - Taiwan

TDG - Transportation of Dangerous Goods

TECIS Inventory

TSCA - Toxic Substances Control Act (United States)

UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods

vPvB - Very Persistent and Very Bioaccumulative

Global Materials Information System

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 use 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.