

## Chemical Safety Data Sheet MSDS / SDS

**8-chloro-6-phenyl-1-(trideuteriomethyl)-4H-[1,2,4]triazolo[4,3-a][1,4]benzodiazepine**

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

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

Product name : 8-chloro-6-phenyl-1-(trideuteriomethyl)-4H-[1,2,4]triazolo[4,3-a][1,4]benzodiazepine  
CBnumber : CB03601394  
CAS : 112393-64-3  
Synonyms : Alprazolam-d3 (exempt preparation);Alprazolam-d3 (1mg/ml in Acetonitrile)

**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

Warning

**Precautionary statements**

P501 Dispose of contents/container to....  
P405 Store locked up.  
P308+P313 IF exposed or concerned: Get medical advice/attention.  
P330 Rinse mouth.  
P301+P312 IF SWALLOWED: call a POISON CENTER or doctor/physician IF you feel unwell.  
P280 Wear protective gloves/protective clothing/eye protection/face protection.  
P270 Do not eat, drink or smoke when using this product.  
P264 Wash skin thoroughly after handling.  
P263 Avoid contact during pregnancy/while nursing.  
P260 Do not breathe dust/fume/gas/mist/vapours/spray.

P202 Do not handle until all safety precautions have been read and understood.

P201 Obtain special instructions before use.

#### **Hazard statements**

H362 May cause harm to breast-fed children

H361 Suspected of damaging fertility or the unborn child

H302 Harmful if swallowed

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

### **Substance**

|              |                                                                                        |
|--------------|----------------------------------------------------------------------------------------|
| Product name | : 8-chloro-6-phenyl-1-(trideuteriomethyl)-4H-[1,2,4]triazolo[4,3-a][1,4]benzodiazepine |
| Synonyms     | : Alprazolam-d3 (exempt preparation);Alprazolam-d3 (1mg/ml in Acetonitrile)            |
| CAS          | : 112393-64-3                                                                          |
| MF           | : C <sub>17</sub> H <sub>10</sub> ClD <sub>3</sub> N <sub>4</sub>                      |
| MW           | : 311.783                                                                              |

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## **SECTION 4: First aid measures**

### **Description of first aid measures**

#### **General information**

Immediately remove any clothing soiled by the product.

Remove breathing apparatus only after contaminated clothing have been completely removed.

In case of irregular breathing or respiratory arrest provide artificial respiration.

#### **After inhalation**

Supply fresh air or oxygen; call for doctor.

In case of unconsciousness place patient stably in side position for transportation.

#### **After skin contact**

Immediately wash with water and soap and rinse thoroughly.

#### **After eye contact**

Rinse opened eye for several minutes under running water. Then consult a doctor.

#### **After swallowing**

Do not induce vomiting; immediately call for medical help.

#### **Information for doctor**

#### **Most important symptoms and effects, both acute and delayed**

No further relevant information available.

#### **Indication of any immediate medical attention and special treatment needed**

No further relevant information available.

## SECTION 5: Firefighting measures

### Extinguishing media

#### Suitable extinguishing agents

CO<sub>2</sub>, extinguishing powder or water spray. Fight larger fires with water spray or alcohol resistant foam.

#### Special hazards arising from the substance or mixture

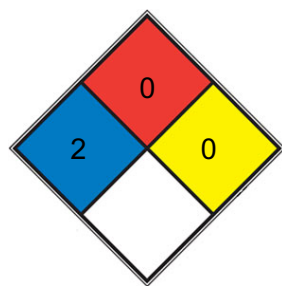
67-56-1 During heating or in case of fire poisonous gases are produced.

#### Advice for firefighters

#### Protective equipment

Mouth respiratory protective device.

#### NFPA 704



■ HEALTH 2 Intense or continued but not chronic exposure could cause temporary incapacitation or possible residual injury (e.g. [diethyl ether](#), ammonium phosphate, iodine)

■ FIRE 0 Materials that will not burn under typical fire conditions, including intrinsically noncombustible materials such as concrete, stone, and sand. Materials that will not burn in air when exposed to a temperature of 820 °C (1,500 °F) for a period of 5 minutes. (e.g. Carbon tetrachloride)

■ REACT 0 Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, [N<sub>2</sub>](#))

□ SPEC.

□ HAZ.

## SECTION 6: Accidental release measures

56.0

| Personal precautions, protective equipment and emergency procedures |  |  |  |  |  |  |  |                    |  |  |    |
|---------------------------------------------------------------------|--|--|--|--|--|--|--|--------------------|--|--|----|
| Mount respiratory protective device.                                |  |  |  |  |  |  |  |                    |  |  |    |
| Wear protective equipment. Keep unprotected persons away.           |  |  |  |  |  |  |  |                    |  |  |    |
|                                                                     |  |  |  |  |  |  |  | (Contd. on page 4) |  |  |    |
|                                                                     |  |  |  |  |  |  |  |                    |  |  | US |

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## Reference to other sections

See Section 7 for information on safe handling.

See Section 8 for information on personal protection equipment.

See Section 13 for disposal information.

## Protective Action Criteria for Chemicals

### PAC-1

67-56-1 Methanol 530 ppm

### PAC-2

67-56-1 Methanol 2,100 ppm

### PAC-3

67-56-1 Methanol 7200\* ppm

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## SECTION 7: Handling and storage

### Handling

#### Precautions for safe handling

Ensure good ventilation/exhaustion at the workplace.

Open and handle receptacle with care.

Prevent formation of aerosols.

#### Information about protection against explosions and fires

Keep ignition sources away - Do not smoke.

Protect against electrostatic charges.

Keep respiratory protective device available.

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

### Storage

Store in accordance with information listed on the product insert.

#### Requirements to be met by storerooms and receptacles

Store in a cool location.

#### Information about storage in one common storage facility

Not required.

#### Further information about storage conditions

Keep receptacle tightly sealed.

Store in cool, dry conditions in well sealed receptacles.

## Specific end use(s)

No further relevant information available.

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## SECTION 8: Exposure controls/personal protection

### Additional information about design of technical systems

No further data; see item 7.

### Control parameters

Components with limit values that require monitoring at the workplace:

| 67-56-1 Methanol |                                                   |
|------------------|---------------------------------------------------|
| PEL              | Long-term value: 260 mg/m <sup>3</sup> , 200 ppm  |
|                  | Short-term value: 325 mg/m <sup>3</sup> , 250 ppm |
| REL              | Long-term value: 260 mg/m <sup>3</sup> , 200 ppm  |
|                  | Skin 56.0                                         |
| TLV              | Short-term value: 250 ppm                         |
|                  | Long-term value: 200 ppm                          |
|                  | Skin; BEI                                         |

| Ingredients with biological limit values: |                                               |
|-------------------------------------------|-----------------------------------------------|
| 67-56-1 Methanol                          |                                               |
| BEI                                       | 15 mg/L                                       |
|                                           | Medium: urine                                 |
|                                           | Time: end of shift                            |
|                                           | Parameter: Methanol (background, nonspecific) |

### Additional information

The lists that were valid during the creation were used as basis.

### Exposure controls

#### Personal protective equipment

#### General protective and hygienic measures

Keep away from foodstuffs, beverages and feed.

Immediately remove all soiled and contaminated clothing.

Wash hands before breaks and at the end of work.

Store protective clothing separately.

Avoid contact with the eyes and skin.

#### Breathing equipment

In case of brief exposure or low pollution use respiratory filter device. In case of intensive or longer exposure use respiratory protective device

that is independent of circulating air.

### **Protection of hands**

Protective gloves

The glove material has to be impermeable and resistant to the product/ the substance/ the preparation.

Due to missing tests no recommendation to the glove material can be given for the product/ the preparation/ the chemical mixture.

Selection of the glove material on consideration of the penetration times, rates of diffusion and the degradation

### **Material of gloves**

The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer. As the product is a preparation of several substances, the resistance of the glove material can not be calculated in advance and has therefore to be checked prior to the application.

### **Penetration time of glove material**

The exact break through time has to be found out by the manufacturer of the protective gloves and has to be observed.

### **Eye protection**

Tightly sealed goggles 56.0

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## **SECTION 9: Physical and chemical properties**

### **Information on basic physicochemical properties**

#### **Appearance**

#### **Physical State**

Liquid

#### **Color**

According to product specification

#### **Odor**

Alcohol-like

#### **Structural Formula**

C<sub>17</sub>H<sub>10</sub>Cl<sub>3</sub>N<sub>4</sub>

#### **Molecular Weight**

311.8 g/mol

#### **Odor Threshold**

Not determined.

#### **Formulation**

A 100 µg/ml solution in methanol

**pH**

Not determined.

**Change in condition****Melting point/Melting range**

-98 °C (-144.4 °F)

**Boiling point/Boiling range**

64.7 °C (148.5 °F)

**Flash point**

11 °C (51.8 °F)

**Flammability (solid,gas)**

Highly flammable.

**Ignition temperature**

455 °C (851 °F)

**Decomposition temperature**

Not determined.

**Auto igniting**

Product is not selfigniting.

**Danger of explosion**

Product is not explosive. However, formation of explosive air/ vapor mixtures are possible.

**Explosion limits**

Lower: 5.5 Vol %

Upper: 44 Vol %

**Vapor Pressure at 20 °C (68 °F)**

128 hPa (96 mm Hg)

**Density at 20 °C (68 °F)**

0.79 g/cm<sup>3</sup> (6.59255 lbs/gal)

**Relative Density**

Not determined.

**Vapor Density**

Not determined.

**Evaporation Rate**

Not determined.

### **Solubility in / Miscibility with**

Chloroform (Sparingly), Methanol (Slightly)

### **Water**

Fully miscible.

### **Partition coefficient (n-octanol/water)**

Not determined.

### **Viscosity**

#### **Dynamic**

Not determined.

#### **Kinematic**

Not determined.

### **Organic solvents**

100.0 %

### **VOC content**

99.99 % 999.9 g/l / 8.34 lb/gal

### **Solids content**

0.0 %

### **Other information**

No information available

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## **SECTION 10: Stability and reactivity**

### **Reactivity**

No further relevant information available.

### **Chemical stability**

### **Thermal decomposition / conditions to be avoided**

No decomposition if used according to specifications.

### **Possibility of hazardous reactions**

No dangerous reactions known.

### **Conditions to avoid**

No further relevant information available.

## Incompatible materials

reducing agents, oxidizing agents

## Hazardous decomposition products

carbon monoxide, carbon dioxide

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# SECTION 11: Toxicological information

## Information on toxicological effects

### Acute toxicity

LD/LC50 values that are relevant for classification:

| Substance / Estimate | Route           | Endpoint | Value                                                                                                                                                                                                                   |
|----------------------|-----------------|----------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 67-56-1 Methanol     | Oral            | LDLO     | 143 mg/kg (hmn)                                                                                                                                                                                                         |
| 67-56-1 Methanol     | Oral            | TDLO     | 5 ml/kg (rat)                                                                                                                                                                                                           |
| 67-56-1 Methanol     | Oral            | LD50     | 5,600 mg/kg (rat)                                                                                                                                                                                                       |
| 67-56-1 Methanol     | Dermal          | LD50     | 15,800 mg/kg (rabbit)                                                                                                                                                                                                   |
| 67-56-1 Methanol     | Inhalative      | LC50/4 h | 64,000 mg/m <sup>3</sup> (rat)                                                                                                                                                                                          |
| 67-56-1 Methanol     | Inhalative      | LC50     | 61,100 mg/m <sup>3</sup> /134 m (mouse)<br>Irritation of skin Irritation 20 mg/24h (rabbit)<br>Irritation (rabbit)<br>Irritation 5.63 mg/kg/exempt preparation (rabbit)<br>Irritation of eyes Irritation 40 mg (rabbit) |
| 67-56-1 Methanol     | Intraperitoneal | TDLO     | 5 mg/kg (rat)                                                                                                                                                                                                           |
| 67-56-1 Methanol     | Intraperitoneal | LD50     | 10,765 mg/kg (mouse)                                                                                                                                                                                                    |
| 67-56-1 Methanol     | Subcutaneous    | LD50     | 143 mg/kg/human (mouse)<br>Data 20 mg/24h (rabbit)                                                                                                                                                                      |

### Primary irritant effect

#### on the skin

No irritant effect.

#### on the eye

No irritating effect.

### Sensitization

No sensitizing effects known.

### Additional toxicological information

The product shows the following dangers according to internally approved calculation methods for preparations

Toxic

## **Carcinogenic categories**

### **IARC (International Agency for Research on Cancer)**

None of the ingredients is listed.

### **NTP (National Toxicology Program)**

None of the ingredients is listed.

### **OSHA-Ca (Occupational Safety & Health Administration)**

None of the ingredients is listed.

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## **SECTION 12: Ecological information**

### **Toxicity**

#### **Aquatic toxicity**

No further relevant information available.

#### **Persistence and degradability**

No further relevant information available.

#### **Behavior in environmental systems**

#### **Bioaccumulative potential**

No further relevant information available.

#### **Mobility in soil**

No further relevant information available.

### **Additional ecological information**

#### **General notes**

Water hazard class 2 (Self-assessment) hazardous for water

Do not allow product to reach ground water, water course or sewage system.

Danger to drinking water if even small quantities leak into the ground.

### **Results of PBT and vPvB assessment**

#### **PBT**

Not applicable.

#### **vPvB**

Not applicable.

#### **PBT:**

Not applicable.

**vPvB:**

Not applicable.

**Other adverse effects**

No further relevant information available.

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## SECTION 13: Disposal considerations

### Waste treatment methods

#### Recommendation

Must not be disposed of together with household garbage. Do not allow product to reach sewage system.

### Uncleaned packagings

#### Recommendation

Disposal must be made according to official regulations.

#### Recommended cleansing agent

Water, if necessary with cleansing agents.

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## SECTION 14: Transport information

### UN-Number

DOT, IMDG, IATA UN1230

### UN proper shipping name

DOT, IATA Methanol solution

IMDG METHANOL solution 56.0

### Transport hazard class(es)

#### DOT

Class: 3 Flammable liquids

Label: 3, 6.1

#### IMDG

Class: 3 Flammable liquids

Label: 3/6.1

#### IATA

Class: 3 Flammable liquids

Label: 3 (6.1)

### Packing group

DOT, IMDG, IATA II

### **Environmental hazards**

Not applicable.

### **Special precautions for user**

Warning: Flammable liquids

### **Hazard identification number (Kemler code)**

336

### **EMS Number**

F-E,S-D

### **Stowage Category**

B

### **Stowage Code**

SW2 Clear of living quarters.

### **Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code**

Not applicable.

### **Transport/Additional information**

#### **DOT:**

#### **Quantity limitations**

On passenger aircraft/rail: 1 L

On cargo aircraft only: 60 L

#### **IMDG:**

#### **Limited quantities (LQ)**

1L

#### **Excepted quantities (EQ)**

Code: E2

Maximum net quantity per inner packaging: 30 ml

Maximum net quantity per outer packaging: 500 ml

#### **IATA:**

#### **Remarks**

When sold in quantities of less than or equal to 1 mL, or 1 g, with an Excepted Quantity Code of E1, E2, E4, or E5, this item meets the De Minimis

Quantities exemption, per IATA 2.6.10.

56.0

Therefore packaging does not have to be labeled as

Dangerous Goods/Excepted Quantity.

## UN "Model Regulation"

UN 1230 METHANOL SOLUTION, 3 (6.1), II

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## SECTION 15: Regulatory information

### Safety, health and environmental regulations/legislation specific for the substance or mixture

No further relevant information available.

#### Sara

|                                                 |                                    |
|-------------------------------------------------|------------------------------------|
| Section 355 (extremely hazardous substances):   | None of the ingredients is listed. |
| Section 313 (Specific toxic chemical listings): | 67-56-1 Methanol                   |
| TSCA (Toxic Substances Control Act):            | 67-56-1 Methanol ACTIVE            |
| Hazardous Air Pollutants 67-56-1 Methanol       |                                    |

#### Proposition 65

|                                                             |                                    |
|-------------------------------------------------------------|------------------------------------|
| Chemicals known to cause cancer:                            | None of the ingredients is listed. |
| Chemicals known to cause reproductive toxicity for females: | None of the ingredients is listed. |
| Chemicals known to cause reproductive toxicity for males:   | None of the ingredients is listed. |
| Chemicals known to cause developmental toxicity:            | 67-56-1 Methanol                   |

#### Carcinogenic categories

|                                        |                                    |
|----------------------------------------|------------------------------------|
| EPA (Environmental Protection Agency): | None of the ingredients is listed. |
|----------------------------------------|------------------------------------|

#### TLV (Threshold Limit Value)

None of the ingredients is listed.

#### NIOSH-Ca (National Institute for Occupational Safety and Health)

None of the ingredients is listed.

#### Chemical safety assessment

A Chemical Safety Assessment has not been carried out.

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## SECTION 16: Other information

### Abbreviations and acronyms

IMDG: International Maritime Code for Dangerous Goods

DOT: US Department of Transportation

IATA: International Air Transport Association

EINECS: European Inventory of Existing Commercial Chemical Substances

ELINCS: European List of Notified Chemical Substances

CAS: Chemical Abstracts Service (division of the American Chemical Society)

NFPA: National Fire Protection Association (USA)

HMS: Hazardous Materials Identification System (USA)

VOC: Volatile Organic Compounds (USA, EU)

LC50: Lethal concentration, 50 percent

LD50: Lethal dose, 50 percent

PBT: Persistent, Bioaccumulative and Toxic vPvB: very Persistent and very Bioaccumulative

NIOSH: National Institute for Occupational Safety

OSHA: Occupational Safety & Health

TLV: Threshold Limit Value

PEL: Permissible Exposure Limit

REL: Recommended Exposure Limit

BEI: Biological Exposure Limit

Flammable Liquids 2: Flammable liquids – Category 2

Acute Toxicity - Oral 3: Acute toxicity – Category 3

Specific Target Organ Toxicity - Single Exposure 1: Specific target organ toxicity (single exposure) – Category 1 56.0

**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.