

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

P201 Obtain special instructions before use.
P202 Do not handle until all safety precautions have been read and understood.
P260 Do not breathe dust/fume/gas/mist/vapours/spray.
P263 Avoid contact during pregnancy/while nursing.
P264 Wash skin thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P280 Wear protective gloves/protective clothing/eye protection/face protection.
P301+P312 IF SWALLOWED: call a POISON CENTER or doctor/physician IF you feel unwell.
P330 Rinse mouth.
P308+P313 IF exposed or concerned: Get medical advice/attention.

P405 Store locked up.

P501 Dispose of contents/container to.....

Hazard statements

H302 Harmful if swallowed

H361 Suspected of damaging fertility or the unborn child

H362 May cause harm to breast-fed children

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	: C17H10ClD3N4
MW	: 311.783

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

CO₂, extinguishing powder or water spray. Fight larger fires with water spray or alcohol resistant foam.

Special hazards arising from the substance or mixture

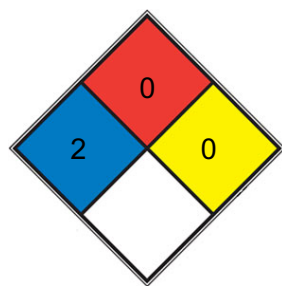
67-56-1 During heating or in case of fire poisonous gases are produced.

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,[N₂](#))

□ SPEC.

□ HAZ.

SECTION 6: Accidental release measures

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

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

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.

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 ³ , 200 ppm
	Short-term value: 325 mg/m ³ , 250 ppm
REL	Long-term value: 260 mg/m ³ , 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

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

C₁₇H₁₀Cl₃N₄

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/cm³ (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

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

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 ³ (rat)
67-56-1 Methanol	Inhalative	LC50	61,100 mg/m ³ /134 m (mouse) Irritation of skin Irritation 20 mg/24h (rabbit) Irritation (rabbit) Irritation 5.63 mg/kg/exempt preparation (rabbit) 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) 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.

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.

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.

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.

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Therefore packaging does not have to be labeled as

Dangerous Goods/Excepted Quantity.

UN "Model Regulation"

UN 1230 METHANOL SOLUTION, 3 (6.1), II

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.
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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.

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.