

Chemical Safety Data Sheet MSDS / SDS

Caffeine-d3 (1-methyl-d3)

Revision Date:2026-09-13 Revision Number:1

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

Product name : Caffeine-d3 (1-methyl-d3)
CBnumber : CB5106910
CAS : 26351-03-1
Synonyms : CICC402;Caffeine-d3 (CRM)

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

P501 Dispose of contents/container to.....
P405 Store locked up.
P330 Rinse mouth.
P321 Specific treatment (see ... on this label).
P301+P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.
P273 Avoid release to the environment.
P270 Do not eat, drink or smoke when using this product.
P264 Wash skin thoroughly after handling.

Hazard statements

H402 Harmful to aquatic life
H301 Toxic if swallowed

SECTION 3: Composition/information on ingredients

Substance

Product name	: Caffeine-d3 (1-methyl-d3)
Synonyms	: CICC402;Caffeine-d3 (CRM)
CAS	: 26351-03-1
MF	: C ₈ H ₇ D ₃ N ₄ O ₂
MW	: 197.21

SECTION 4: First aid measures

Description of first aid measures

General information

Immediately remove any clothing soiled by the product.

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

After inhalation

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

May cause anemia, cough, CNS depression, drowsiness, headache, heart damage, lassitude (weakness, exhaustion), liver damage, narcosis, reproductive effects, teratogenic effects.

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

Use fire fighting measures that suit the environment.

A solid water stream may be inefficient.

Special hazards arising from the substance or mixture

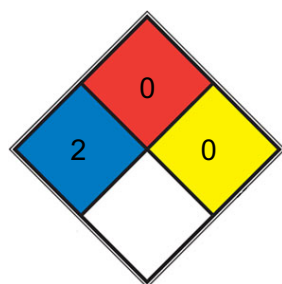
No further relevant information available.

Advice for firefighters

Protective equipment

No special measures required.

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

Personal precautions, protective equipment and emergency procedures

Not required.

Environmental precautions

Do not allow to enter sewers/ surface or ground water.

Methods and material for containment and cleaning up

Dispose contaminated material as waste according to item 13.

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

Substance is not listed.

PAC-2

Substance is not listed.

PAC-3

Substance is not listed.

SECTION 7: Handling and storage

Handling

Precautions for safe handling

Thorough dedusting.

Information about protection against explosions and fires

No special measures required.

Conditions for safe storage, including any incompatibilities

Keep container tightly closed.

Store in accordance with information listed on the product insert.

Storage

Store in accordance with information listed on the product insert.

Requirements to be met by storerooms and receptacles

No special requirements.

Information about storage in one common storage facility

Not required.

Further information about storage conditions

None.

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

Not required.

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.

Breathing equipment

Not required.

Protection of hands

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.

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

Not required.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Appearance

white powder

Physical State

neat solid

Color

Not determined.

Odor

Characteristic

Structural Formula

C₈H₇D₃N₄O₂

Molecular Weight

197.2 g/mol

Odor Threshold

Not determined.

pH

Not applicable.

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

Undetermined.

Boiling point/Boiling range

Undetermined.

Flash point

Not applicable.

Flammability (solid,gas)

Product is not flammable.

Decomposition temperature

Not determined.

Auto igniting

Not determined.

Danger of explosion

Product does not present an explosion hazard.

Explosion limits

Lower: Not determined.

Upper: Not determined.

Vapor Pressure

Not applicable.

Density

Not determined.

Relative Density

Not determined.

Vapor Density

Not applicable.

Evaporation Rate

Not applicable.

Solubility in / Miscibility with

DMF: 10 mg/ml; DMSO: 2 mg/ml; Ethanol: 0.2 mg/ml; PBS (pH 7.2): 5 mg/ml

Water

Not determined.

Partition coefficient (n-octanol/water)

Not determined.

Viscosity

Dynamic

Not applicable.

Kinematic

Not applicable.

SOLUBILITY

DMF: 10 mg/ml; DMSO: 2 mg/ml; Ethanol: 0.2 mg/ml; PBS (pH 7.2): 5 mg/ml

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

strong oxidizing agents

Hazardous decomposition products

carbon oxides, nitrogen oxides

SECTION 11: Toxicological information

Information on toxicological effects**Primary irritant effect****on the skin**

No irritant effect.

on the eye

No irritating effect.

Sensitization

No sensitizing effects known.

Additional toxicological information**Carcinogenic categories****IARC (International Agency for Research on Cancer)**

Substance is not listed.

NTP (National Toxicology Program)

Substance is not listed.

OSHA-Ca (Occupational Safety & Health Administration)

Substance is not 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 1 (Self-assessment) slightly hazardous for water

Do not allow undiluted product or large quantities of it to reach ground water, water course or sewage system.

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.

SECTION 14: Transport information

UN-Number

DOT, IMDG, IATA UN2811

UN proper shipping name

DOT Toxic solids, organic, n.o.s. (Caffeine-d3)

IMDG TOXIC SOLID, ORGANIC, N.O.S. (Caffeine-d3)

IATA Toxic solid, organic, n.o.s. (Caffeine-d3)

Transport hazard class(es)

DOT

Class: 6.1 Toxic substances

Label: 6.1

IMDG, IATA

Class: 6.1 Toxic substances

Label: 6.1

Packing group

DOT, IMDG, IATA III

Environmental hazards

Not applicable.

Special precautions for user Warning: Toxic substances

Warning: Toxic substances

Hazard identification number (Kemler code)

60

EMS Number

F-A,S-A

Stowage Category

A

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: 100 kg

On cargo aircraft only: 200 kg

IMDG:

Limited quantities (LQ)

5 kg

Excepted quantities (EQ)

Code: E1

Maximum net quantity per inner packaging: 30 g

Maximum net quantity per outer packaging: 1000 g

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.

Therefore packaging does not have to be labeled as Dangerous Goods/Excepted Quantity.

UN "Model Regulation"

UN 2811 TOXIC SOLID, ORGANIC, N.O.S.

(CAFFEINE-D3), 6.1, III

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):	Substance is not listed.
Section 313 (Specific toxic chemical listings):	Substance is not listed.
TSCA (Toxic Substances Control Act):	Substance is not listed.
Hazardous Air Pollutants:	Substance is not listed.

Proposition 65

Chemicals known to cause cancer:	Substance is not listed.
Chemicals known to cause reproductive toxicity for females:	Substance is not listed.
Chemicals known to cause reproductive toxicity for males:	Substance is not listed.
Chemicals known to cause developmental toxicity:	Substance is not listed.

Chemicals known to cause cancer

Substance is not listed.

Chemicals known to cause reproductive toxicity for females

Substance is not listed.

Chemicals known to cause reproductive toxicity for males

Substance is not listed.

Chemicals known to cause developmental toxicity

Substance is not listed.

Carcinogenic categories

EPA (Environmental Protection Agency):	Substance is not listed.
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TLV (Threshold Limit Value)

Substance is not listed.

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

Substance is not 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

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

NFPA: National Fire Protection Association (USA)

HMS: Hazardous Materials Identification System (USA)

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

Acute Toxicity - Oral 3: Acute toxicity – Category 3

Aquatic Acute 3: Hazardous to the aquatic environment - acute aquatic hazard – Category 3

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.