

Chemical Safety Data Sheet MSDS / SDS

Caffeine

Revision Date:2026-06-27 Revision Number:1

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

Product identifier

Product name : Caffeine
CBnumber : CB0202769
CAS : 58-08-2
EINECS Number : 200-362-1
Synonyms : caffeine,caffine

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

No data available

Hazard statementsH302 Harmful if swallowed

SECTION 3: Composition/information on ingredients

Substance

Product name : Caffeine
Synonyms : caffeine,caffine

CAS	: 58-08-2
EC number	: 200-362-1
MF	: C8H10N4O2
MW	: 194.19

SECTION 4: First aid measures

Description of first aid measures

General information

Symptoms of poisoning may even occur after several hours; therefore medical observation for at least 48 hours after the accident.

After inhalation

Supply fresh air; consult doctor in case of complaints.

After skin contact

Generally the product does not irritate the skin.

After eye contact

Rinse opened eye for several minutes under running water.

After swallowing

Immediately call a doctor.

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

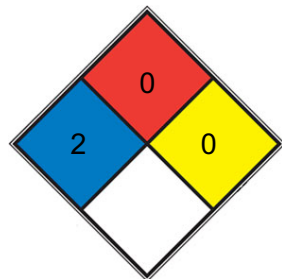
No further relevant information available.

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

No special precautions are necessary if used correctly.

Avoid breathing dust/fume/gas/mist/vapours/spray.

Avoid prolonged or repeated exposure.

Keep away from sources of ignition.

Take precautionary measures against static discharge.

Information about protection against explosions and fires

No special measures required.

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

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.

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

Physical State

Solid

Color

Silky white or white

Odor

Characteristic

Structural Formula

C₈H₁₀N₄O₂

Molecular Weight

194.2 g/mol

Odor Threshold

Not determined.

pH

pH (10g/l, 25°C) : 5.5~6.5

Change in condition

Melting point/Melting range

235–237 °C (455–458.6 °F)

Boiling point/Boiling range

178 °C (352.4 °F)

Flash point

178°C

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

20 hPa (80 °C)

Density at 20 °C (68 °F)

1.23 g/cm³ (10.26435 lbs/gal)

Relative Density

1.23

Vapor Density

Not applicable.

Evaporation Rate

Not applicable.

Solubility in / Miscibility with

Sparingly soluble in water, freely soluble in boiling water, slightly soluble in ethanol (96 per cent). It dissolves in concentrated solutions of alkali benzoates or salicylates.

Water

Soluble.

Partition coefficient (n-octanol/water)

Not determined.

Viscosity**Dynamic**

Not applicable.

Kinematic

Not applicable.

SOLUBILITY

DMF: 10 mg/ml; DMSO: 3 mg/ml; Ethanol: 0.2 mg/ml; PBS (pH 7.2): 5 mg/ml

VOC content: 0.00 %

Solids content: 100.0 %

Water solubility

20 g/L (20 °C)

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 dioxide, carbon monoxide, nitrogen oxides

SECTION 11: Toxicological information

RTECS Number

KQ6300000

Information on toxicological effects

Acute toxicity

LD/LC50 values that are relevant for classification:

Substance / Estimate	Route	Endpoint	Value
ATE (Acute Toxicity Estimate)	Oral	LD50	192 mg/kg (rat)
58-08-2 Caffeine	Oral	LDLO	400 mg/kg (wmn)
58-08-2 Caffeine	Oral	LD50	192 mg/kg (rat)
58-08-2 Caffeine	Oral	TDLO	140 mg/kg (chd)
58-08-2 Caffeine	Intraperitoneal	LD50	240 mg/kg (rat)
58-08-2 Caffeine	Subcutaneous	LD50	170 mg/kg (rat)

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

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 (Assessment by list): 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.

Recommended cleansing agent

Water, if necessary with cleansing agents.

SECTION 14: Transport information

UN-Number

DOT, IMDG, IATA UN2811

UN proper shipping name

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

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

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

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

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), 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):	ACTIVE
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.

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.

ACTIVE

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

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

Acute Tox. 4: Acute toxicity – Category 4

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.