

Safety Data Sheet

according to Regulation (EC) No 1907/2006 (REACH)
Classifications according to Regulation (EC) No 1272/2008.
Printdate 16 Aug 2022

1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

1.1. Product name:

13C3-Caffeine

1.1. Catalog No.:

681491

1.2. Relevant identified uses of the substance or mixture

Identified: Laboratory chemical
uses: R&D

1.3. Uses advised against:

HPC Standards GmbH
Am Wieseneck 7

04451 Cunnersdorf
Deutschland

Tel. +49 34291 3372-36
Fax. +49 34291 3372-39
contact@hpc-standards.com

1.4. Emergency telephone number

HPC Standards Tel. +49 34291 3372-36
This number is only available during office hours.

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture
Classification according to Regulation (EC) No 1272/2008
Flammable liquids (Category 2), H225
Acute toxicity, Oral (Category 3), H301
Acute toxicity, Inhalation (Category 3), H331
Acute toxicity, Dermal (Category 3), H311
Specific target organ toxicity - single exposure (Category 1), H370
For the full text of the H-Statements mentioned in this Section, see Section 16.
Classification according to EU Directives 67/548/EEC or 1999/45/EC
F Highly flammable R11
T Toxic R23/24/25, R39/23/24/25

2.2. Label elements

2.2.1. Pictogram



2.2.2.

Signal word Danger

Hazard statement(s)

H225 Highly flammable liquid and vapour.

H301 + H311 + H331 Toxic if swallowed, in contact with skin or if inhaled

H370 Causes damage to organs.

Precautionary statement(s)

P210 Keep away from heat/sparks/open flames/hot surfaces. - No smoking.

P260 Do not breathe dust/ fume/ gas/ mist/ vapours/ spray.

P280 Wear protective gloves/ protective clothing.

P301 + P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/ physician.

P311 Call a POISON CENTER or doctor/ physician.

Supplemental Hazard Statements

none

2.3 Other hazards

This substance is not considered to be persistent, bioaccumulating nor toxic (PBT)., This substance is not considered to be very persistent nor very bioaccumulating (vPvB).

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms : Methyl alcohol

Formula : CH₄O

Molecular Weight : 32,04 g/mol

CAS-No. : 67-56-1

EC-No. : 200-659-6

Index-No. : 603-001-00-X

Registration number : 01-2119433307-44-XXXX

Hazardous ingredients according to Regulation (EC) No 1272/2008

Component Classification Concentration

Methanol

CAS-No.

EC-No.

Index-No.

Registration number

67-56-1

200-659-6

603-001-00-X

01-2119433307-44-XXXX

Flam. Liq. 2; Acute Tox. 3;

STOT SE 1; H225, H301 +

H311 + H331, H370

<= 100 %

Hazardous ingredients according to Directive 1999/45/EC

Component Classification Concentration

Methanol

CAS-No.

EC-No.

Index-No.

Registration number

67-56-1

200-659-6

603-001-00-X

01-2119433307-44-XXXX

F, T, R11 - R23/24/25 -

R39/23/24/25

<= 100 %

3.1.1. Formula

C₈H₁₀N₄O₂

3.1.2. Molecular Weight (g/mol)

197.22

3.1.3. CAS-No.

78072-66-9

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice

Consult a physician. Show this safety data sheet to the doctor in attendance.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

In case of eye contact

Flush eyes with water as a precaution.

If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

no data available

5. FIRE-FIGHTING MEASURES

5.1 Extinguishing media

Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

5.3 Advice for firefighters

Wear self contained breathing apparatus for fire fighting if necessary.

5.4 Further information

Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Wear respiratory protection. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.

6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up

Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

6.4 Reference to other sections

For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.

Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

7.2 Conditions for safe storage, including any incompatibilities

Store in cool place. Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Recommended storage temperature: 2 - 8 °C

7.3 Specific end use(s)

no data available

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters

8.2 Exposure controls

Appropriate engineering controls

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

Personal protective equipment

Eye/face protection

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

Skin protection

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 EU Directive 89/686/EEC and the standard EN 374 derived from it.

Body Protection

Complete suit protecting against chemicals, Flame retardant antistatic protective clothing, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type AXBEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a) Appearance Form: liquid

Colour: colourless

b) Odour pungent

c) Odour Threshold no data available

d) pH no data available

e) Melting point/freezing point

Melting point/range: -98 °C

f) Initial boiling point and boiling range

64,7 °C

g) Flash point 9,7 °C - closed cup

h) Evaporation rate no data available

i) Flammability (solid, gas) no data available

j) Upper/lower flammability or

explosive limits

Upper explosion limit: 36 %(V)

Lower explosion limit: 6 %(V)

k) Vapour pressure 130,3 hPa at 20,0 °C

546,6 hPa at 50,0 °C

169,27 hPa at 25,0 °C

l) Vapour density 1,11

m) Relative density 0,791 g/mL at 25 °C

n) Water solubility completely miscible

o) Partition coefficient: noctanol/ water

log Pow: -0,77

p) Auto-ignition

temperature

455,0 °C at 1.013 hPa

q) Decomposition

temperature

no data available

r) Viscosity no data available

s) Explosive properties Not explosive

t) Oxidizing properties The substance or mixture is not classified as oxidizing.

9.2 Other safety information

Minimum ignition energy 0,14 mJ

Conductivity < 1 µS/cm

Relative vapour density 1,11

10. STABILITY AND REACTIVITY

10.1 Reactivity

no data available

10.2 Chemical stability

no data available

10.3 Possibility of hazardous reactions

no data available

10.4 Conditions to avoid

Heat, flames and sparks. Extremes of temperature and direct sunlight.

10.5 Incompatible materials

Acids, Oxidizing agents, Alkali metals, Acid chlorides, Acid anhydrides, Reducing agents

10.6 Hazardous decomposition products

Other decomposition products - no data available

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LDLO Oral - Human - 143 mg/kg

Remarks: Lungs, Thorax, or Respiration: Dyspnea. Ingestion may cause gastrointestinal irritation, nausea, vomiting and diarrhoea.

LD50 Oral - rat - 1.187 - 2.769 mg/kg

LC50 Inhalation - rat - 4 h - 128,2 mg/l

LC50 Inhalation - rat - 6 h - 87,6 mg/l

LD50 Dermal - rabbit - 17.100 mg/kg

Skin corrosion/irritation

Skin - rabbit

Result: No skin irritation

Serious eye damage/eye irritation

Eyes - rabbit

Result: No eye irritation

Respiratory or skin sensitisation

Maximisation Test - guinea pig

Does not cause skin sensitisation.

(OECD Test Guideline 406)

Germ cell mutagenicity

Ames test

S. typhimurium

Result: negative

in vitro assay

fibroblast

Result: negative

Mutation in mammalian somatic cells.

Mutagenicity (in vivo mammalian bone-marrow cytogenetic test, chromosomal analysis)

mouse - male and female

Result: negative

Carcinogenicity

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

Reproductive toxicity

Damage to fetus not classifiable

Fertility classification not possible from current data.

Specific target organ toxicity - single exposure

Causes damage to organs.

Specific target organ toxicity - repeated exposure

The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

Aspiration hazard

No aspiration toxicity classification

Additional Information

RTECS: PC1400000

Methyl alcohol may be fatal or cause blindness if swallowed.

Effects due to ingestion may include: Headache, Dizziness, Drowsiness, metabolic acidosis, Coma, Seizures.

Symptoms may be delayed., Damage of the: Liver, Kidney

12. ECOLOGICAL INFORMATION

12.1 Toxicity

no data available

12.2 Persistence and degradability

no data available

12.3 Bioaccumulative potential

no data available

12.4 Mobility in soil

no data available

12.5 Results of PBT and vPvB assessment

no data available

12.6 Other adverse effects

no data available

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product

Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company.

Contaminated packaging

Dispose of as unused product.

14. TRANSPORT INFORMATION

14.1 UN number

ADR/RID: 1230 IMDG: 1230 IATA: 1230

14.2 UN proper shipping name

ADR/RID: METHANOL

IMDG: METHANOL

IATA: Methanol

14.3 Transport hazard class(es)

ADR/RID: 3 (6.1) IMDG: 3 (6.1) IATA: 3 (6.1)

14.4 Packaging group

ADR/RID: II IMDG: II IATA: II

14.5 Environmental hazards

ADR/RID: no IMDG Marine Pollutant: no IATA: no

14.6 Special precautions for user

no data available

15. REGULATORY INFORMATION

This safety datasheet complies with the requirements of Regulation (EC) No. 1907/2006.

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

no data available

15.2 Chemical Safety Assessment

no data available

16. OTHER INFORMATION

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. For lab use only!