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

1.1 Product identifiers

Product name: Caffeine

Product Number: W222402
Brand: Aldrich
Index-No.: 613-086-00-5
CAS-No.: 58-08-2

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses: Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company: Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone: +1 314 771-5765
Fax: +1 800 325-5052

1.4 Emergency telephone

Emergency Phone #: 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Acute toxicity, Oral (Category 4), H302
Short-term (acute) aquatic hazard (Category 3), H402

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram

Signal word: Warning
Hazard statement(s): Harmful if swallowed.
**Harmful to aquatic life.**

**Precautionary statement(s)**
- **P264** Wash skin thoroughly after handling.
- **P270** Do not eat, drink or smoke when using this product.
- **P273** Avoid release to the environment.
- **P301 + P312 + P330** IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.
- **P501** Dispose of contents/ container to an approved waste disposal plant.

2.3 **Hazards not otherwise classified (HNOC) or not covered by GHS** - none

### SECTION 3: Composition/information on ingredients

3.1 **Substances**

**Synonyms:** 1,3,7-Trimethylxanthine

**Formula:** C₈H₁₀N₄O₂

**Molecular weight:** 194.19 g/mol

**CAS-No.:** 58-08-2

**EC-No.:** 200-362-1

**Index-No.:** 613-086-00-5

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Caffeine</td>
<td>Acute Tox. 4; Aquatic Acute 3; H302, H402</td>
<td>&lt;= 100 %</td>
</tr>
</tbody>
</table>

For the full text of the H-Statements mentioned in this Section, see Section 16.

### SECTION 4: First aid measures

4.1 **Description of first-aid measures**

**General advice**
Consult a physician. Show this material safety data sheet to the doctor in attendance. Move out of dangerous area.

**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. Consult a physician.

**In case of eye contact**
Flush eyes with water as a precaution.

**If swallowed**
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

SECTION 5: Firefighting 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
Nitrogen oxides (NOx)

5.3 Advice for firefighters
Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information
No data available

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures
Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Avoid breathing dust. For personal protection see section 8.

6.2 Environmental precautions
Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up
Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

6.4 Reference to other sections
For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling
Advice on safe handling
Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Advice on safe handling
Further processing of solid materials may result in the formation of combustible dusts. The potential for combustible dust formation should be taken into consideration before additional processing occurs.

Advice on protection against fire and explosion
Provide appropriate exhaust ventilation at places where dust is formed.
Hygiene measures
Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday. For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions
Keep container tightly closed in a dry and well-ventilated place.
Storage class (TRGS 510): 13: Non Combustible Solids

7.3 Specific end use(s)
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters
Contains no substances with occupational exposure limit values.

8.2 Exposure controls

Appropriate engineering controls
Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye/face protection
Safety glasses with side-shields conforming to EN166 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.

Full contact
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested:Dermatril® (KCL 740 / Aldrich Z677272, Size M)

Splash contact
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested:Dermatril® (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374
If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our
customers. It should not be construed as offering an approval for any specific use scenario.

**Body Protection**
Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

**Respiratory protection**
For nuisance exposures use type P95 (US) or type P1 (EU EN 143) particle respirator. For higher level protection use type OV/AG/P99 (US) or type ABEK-P2 (EU EN 143) respirator cartridges. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

**Control of environmental exposure**
Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

### SECTION 9: Physical and chemical properties

#### 9.1 Information on basic physical and chemical properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>a)</strong> Appearance</td>
<td>Form: Crystalline powder</td>
</tr>
<tr>
<td></td>
<td>Color: colorless</td>
</tr>
<tr>
<td><strong>b)</strong> Odor</td>
<td>odorless</td>
</tr>
<tr>
<td><strong>c)</strong> Odor Threshold</td>
<td>No data available</td>
</tr>
<tr>
<td><strong>d)</strong> pH</td>
<td>No data available</td>
</tr>
<tr>
<td><strong>e)</strong> Melting point/freezing point</td>
<td>Melting point/range: 234 - 236.5 °C (453 - 457.7 °F) - lit.</td>
</tr>
<tr>
<td><strong>f)</strong> Initial boiling point and boiling range</td>
<td>No data available</td>
</tr>
<tr>
<td><strong>g)</strong> Flash point</td>
<td>()No data available</td>
</tr>
<tr>
<td><strong>h)</strong> Evaporation rate</td>
<td>No data available</td>
</tr>
<tr>
<td><strong>i)</strong> Flammability (solid, gas)</td>
<td>The product is not flammable.</td>
</tr>
<tr>
<td><strong>j)</strong> Upper/lower flammability or explosive limits</td>
<td>No data available</td>
</tr>
<tr>
<td><strong>k)</strong> Vapor pressure</td>
<td>No data available</td>
</tr>
<tr>
<td><strong>l)</strong> Vapor density</td>
<td>No data available</td>
</tr>
<tr>
<td><strong>m)</strong> Relative density</td>
<td>1.23 at 18 °C (64 °F)</td>
</tr>
<tr>
<td><strong>n)</strong> Water solubility</td>
<td>18.7 g/l at 16 °C (61 °F)</td>
</tr>
<tr>
<td><strong>o)</strong> Partition coefficient: n-octanol/water</td>
<td>log Pow: -0.091 at 23 °C (73 °F) - Bioaccumulation is not expected.</td>
</tr>
<tr>
<td><strong>p)</strong> Autoignition temperature</td>
<td>No data available</td>
</tr>
<tr>
<td><strong>q)</strong> Decomposition temperature</td>
<td>No data available</td>
</tr>
<tr>
<td><strong>r)</strong> Viscosity</td>
<td>No data available</td>
</tr>
</tbody>
</table>
s) Explosive properties  No data available

9.2 Other safety information
Dissociation constant  10.4 at 40 °C (104 °F)

SECTION 10: Stability and reactivity

10.1 Reactivity
No data available

10.2 Chemical stability
Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions
No data available

10.4 Conditions to avoid
No data available

10.5 Incompatible materials
Strong oxidizing agents

10.6 Hazardous decomposition products
In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity
LD50 Oral - Rat - male and female - 367.7 mg/kg
(OECD Test Guideline 401)
Remarks:
(Regulation (EC) No 1272/2008, Annex VI)
LC50 Inhalation - Rat - male and female - 4 h - 4.94 mg/l
(OECD Test Guideline 403)
LD50 Dermal - Rat - male and female - > 2,000 mg/kg
(OECD Test Guideline 402)
No data available

Skin corrosion/irritation
Skin - Rabbit
Result: No skin irritation - 4 h
(OECD Test Guideline 404)

Serious eye damage/eye irritation
Eyes - Rabbit
Result: No eye irritation
(OECD Test Guideline 405)

Respiratory or skin sensitization
Local lymph node assay (LLNA) - Mouse
Result: negative  
(OECD Test Guideline 429)

**Germ cell mutagenicity**  
In vitro mammalian cell gene mutation test  
mouse lymphoma cells  
Result: negative  
Chromosome aberration test in vitro  
Human lymphocytes  
Result: negative  
Ames test  
Escherichia coli/Salmonella typhimurium  
Result: negative  
Chromosome aberration test in vitro  
Chinese hamster lung cells  
Result: positive

Mouse - male  
Result: negative  
Remarks:  
(ECHA)

Human  
Result: negative  
Remarks:  
(ECHA)

Mouse - male  
Result: negative  
Remarks:  
(ECHA)

OECD Test Guideline 474  
Mouse - male and female - Red blood cells (erythrocytes)  
Result: Positive results were obtained in some in vivo tests.

**Carcinogenicity**

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

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA’s list of regulated carcinogens.

**Reproductive toxicity**

No data available

**Specific target organ toxicity - single exposure**

No data available

**Specific target organ toxicity - repeated exposure**

No data available

Aspiration hazard  
No data available
11.2 Additional Information

Repeated dose toxicity - Mouse - male and female - Oral - 90 d - NOAEL (No observed adverse effect level) - 167.4 - 179.4 mg/kg

Remarks:
(ECHA)

RTECS: EV6475000

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

After absorption of toxic quantities:

Diarrhea
Vomiting
agitation
Headache

Systemic effects:

drop in blood pressure
tachycardia

Handle in accordance with good industrial hygiene and safety practice.

Liver - Irregularities - Based on Human Evidence

Liver - Irregularities - Based on Human Evidence

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish static test LC50 - Leuciscus idus (Golden orfe) - ca. 87 mg/l - 96 h (DIN 38412 part 15)
static test NOEC - Leuciscus idus (Golden orfe) - 46 mg/l - 96 h (DIN 38412 part 15)

Toxicity to daphnia and other aquatic invertebrates static test EC50 - Daphnia magna (Water flea) - 182 mg/l - 48 h (DIN 38412)

Toxicity to algae static test ErC50 - Desmodesmus subspicatus (green algae) - > 100 mg/l - 72 h (OECD Test Guideline 201)
static test NOEC - Desmodesmus subspicatus (green algae) - 6.25 mg/l - 72 h (OECD Test Guideline 201)

Toxicity to bacteria EC50 - activated sludge - > 1,000 mg/l - 3 h (OECD Test Guideline 209)

12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 22 d

Aldrich - W222402
Result: 90 - 100 % - Readily biodegradable.
(OECD Test Guideline 301A)

12.3 Bioaccumulative potential
No data available

12.4 Mobility in soil
No data available

12.5 Results of PBT and vPvB assessment
PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects
An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.
Harmful to aquatic life.
Discharge into the environment must be avoided.

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product
Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

Contaminated packaging
Dispose of as unused product.

SECTION 14: Transport information

DOT (US)
Not dangerous goods

IMDG
Not dangerous goods

IATA
Not dangerous goods

Further information
Not classified as dangerous in the meaning of transport regulations.

SECTION 15: Regulatory information

SARA 302 Components
No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components
This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

**SARA 311/312 Hazards**
Acute Health Hazard, Chronic Health Hazard

**Massachusetts Right To Know Components**
No components are subject to the Massachusetts Right to Know Act.

No components are subject to the Massachusetts Right to Know Act.

**Pennsylvania Right To Know Components**

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>Caffeine</td>
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**New Jersey Right To Know Components**

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**SECTION 16: Other information**

**Further information**
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