1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name : Caffeine
Product Number : C0750
Brand : Sigma-Aldrich
Index-No. : 613-086-00-5
REACH No. : A registration number is not available for this substance as the substance or its uses are exempted from registration, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.
CAS-No. : 58-08-2

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

Identified uses : Laboratory chemicals, Manufacture of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO  63103
USA
Telephone : +1 800-325-5832
Fax : +1 800-325-5052

1.4 Emergency telephone number

Emergency Phone # : (314) 776-6555

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

2.2 GHS Label elements, including precautionary statements

Pictogram

<table>
<thead>
<tr>
<th>Signal word</th>
<th>Hazard statement(s)</th>
<th>Precautionary statement(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Warning</td>
<td>H302</td>
<td>P264: Wash skin thoroughly after handling.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>P270: Do not eat, drink or smoke when using this product.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>P301 + P312: IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>P330: Rinse mouth.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>P501: Dispose of contents/container to an approved waste disposal plant.</td>
</tr>
</tbody>
</table>

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none
3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms: 1,3,7-Trimethylxanthine

Formula: \( \text{C}_8\text{H}_{10}\text{N}_4\text{O}_2 \)
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; H302</td>
<td>90 - 100 %</td>
</tr>
</tbody>
</table>

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

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. 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

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

no data available

5.3 Advice for firefighters

Wear self contained breathing apparatus for fire fighting if necessary.

5.4 Further information

no data available

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Avoid breathing dust.
For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains.
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.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling
Avoid contact with skin and eyes. Avoid formation of dust and aerosols.
Provide appropriate exhaust ventilation at places where dust is formed.
For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities
Keep container tightly closed in a dry and well-ventilated place.
Keep in a dry place.

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

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters
Components 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 CE 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
Do not let product enter drains.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a) Appearance  
   Form: powder  
   Colour: white

b) Odour  
   odourless

c) Odour Threshold  
   no data available

d) pH  
   5.5 - 6.5 at 10 g/l at 20 °C (68 °F)

e) Melting point/freezing point  
   Melting point/range: 234 - 236.5 °C (453 - 457.7 °F) - lit.

f) Initial boiling point and boiling range  
   no data available

g) Flash point  
   no data available

h) Evaporation rate  
   no data available

i) Flammability (solid, gas)  
   no data available

j) Upper/lower flammability or explosive limits  
   no data available

k) Vapour pressure  
   20 hPa (15 mmHg) at 89 °C (192 °F)

l) Vapour density  
   no data available

m) Relative density  
   1.230 g/cm3 at 18 °C (64 °F)

n) Water solubility  
   18.7 g/l at 16 °C (61 °F)

o) Partition coefficient: n-octanol/water  
   log Pow: -0.091 at 23 °C (73 °F)

p) Auto-ignition temperature  
   no data available

q) Decomposition temperature  
   no data available

r) Viscosity  
   no data available

s) Explosive properties  
   no data available

t) Oxidizing properties  
   no data available

9.2 Other safety information

Bulk density  
   220 kg/m3

Dissociation constant  
   10.4 at 40 °C (104 °F)

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
Other decomposition products - no data available
In the event of fire: see section 5

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)

LC50 Inhalation - rat - male and female - 4.94 mg/l
(Calculation method)

LD50 Dermal - rat - male and female - > 2,000 mg/kg
no data available

Skin corrosion/irritation
Skin - rabbit
Result: No skin irritation
(OECD Test Guideline 404)

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

Respiratory or skin sensitisation
- mouse
Result: Did not cause sensitisation on laboratory animals.

Germ cell mutagenicity
rat
Kidney
Micronucleus test

mouse
Micronucleus test

Carcinogenicity
IARC: 3 - Group 3: Not classifiable as to its carcinogenicity to humans (Caffeine)

ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

NTP: No component 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 identified as a carcinogen or potential carcinogen by OSHA.

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

Additional Information
RTECS: EV6475000
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.
Liver - Irregularities - Based on Human Evidence
Liver - Irregularities - Based on Human Evidence

12. ECOLOGICAL INFORMATION

12.1 Toxicity
Toxicity to fish
LC50 - Leuciscus idus (Golden orfe) - 87 mg/l - 96 h
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 - Desmodesmus subspicatus (green algae) - > 100 mg/l - 72 h
(OECD Test Guideline 201)

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
PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects
no data available

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods
Product
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. Offer surplus and non-recyclable solutions to a licensed disposal company.

Contaminated packaging
Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)
Not dangerous goods

IMDG
Not dangerous goods

IATA
Not dangerous goods

15. REGULATORY INFORMATION

REACH No.: A registration number is not available for this substance as the substance...
or its uses are exempted from registration, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

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

SARA 313 Components
SARA 313: 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.

Pennsylvania Right To Know Components

<table>
<thead>
<tr>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>58-08-2</td>
<td></td>
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New Jersey Right To Know Components

<table>
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<tbody>
<tr>
<td>58-08-2</td>
<td></td>
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</tbody>
</table>

California Prop. 65 Components
This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.

<table>
<thead>
<tr>
<th>Acute Tox.</th>
<th>Acute toxicity</th>
</tr>
</thead>
<tbody>
<tr>
<td>H302</td>
<td>Harmful if swallowed.</td>
</tr>
</tbody>
</table>

HMIS Rating

<table>
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<th>Health hazard:</th>
<th>2</th>
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<tbody>
<tr>
<td>Chronic Health Hazard:</td>
<td>*</td>
</tr>
<tr>
<td>Flammability:</td>
<td>0</td>
</tr>
<tr>
<td>Physical Hazard</td>
<td>0</td>
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</tbody>
</table>

NFPA Rating

<table>
<thead>
<tr>
<th>Health hazard:</th>
<th>2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fire Hazard:</td>
<td>0</td>
</tr>
<tr>
<td>Reactivity Hazard:</td>
<td>0</td>
</tr>
</tbody>
</table>

Further information
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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. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Preparation Information
Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

Version: 4.8  Revision Date: 02/26/2014  Print Date: 02/27/2014