

## SAFETY DATA SHEET

Version 5.5  
Revision Date 06/13/2014  
Print Date 01/23/2017

---

**1. PRODUCT AND COMPANY IDENTIFICATION****1.1 Product identifiers**

Product name : Caffeine  
  
Product Number : C53  
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, 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 # : +1-703-527-3887 (CHEMTREC)

---

**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



Signal word

Warning

Hazard statement(s)

H302

Harmful if swallowed.

Precautionary statement(s)

P264

Wash skin thoroughly after handling.

P270

Do not eat, drink or smoke when using this product.

P301 + P312

IF SWALLOWED: Call a POISON CENTER or doctor/ physician if you feel unwell.

P330

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**

---

**3. COMPOSITION/INFORMATION ON INGREDIENTS****3.1 Substances**

Aldrich - C53

Synonyms : 1,3,7-Trimethylxanthine  
Formula : C<sub>8</sub>H<sub>10</sub>N<sub>4</sub>O<sub>2</sub>  
Molecular Weight : 194.19 g/mol  
CAS-No. : 58-08-2  
EC-No. : 200-362-1  
Index-No. : 613-086-00-5

#### Hazardous components

Component	Classification	Concentration
<b>Caffeine</b>		
	Acute Tox. 4; H302	90 - 100 %

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: crystalline, powder<br>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/cm <sup>3</sup> 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/m <sup>3</sup>  |
| 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

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****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

	CAS-No.	Revision Date
Caffeine	58-08-2	

### New Jersey Right To Know Components

	CAS-No.	Revision Date
Caffeine	58-08-2	

### 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.

Acute Tox.	Acute toxicity
H302	Harmful if swallowed.

### HMIS Rating

Health hazard:	2
Chronic Health Hazard:	*
Flammability:	0
Physical Hazard	0

### NFPA Rating

Health hazard:	2
Fire Hazard:	0
Reactivity Hazard:	0

### Further information

Copyright 2014 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only. 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](http://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: 5.5

Revision Date: 06/13/2014

Print Date: 01/23/2017