

### 1. PRODUCT AND COMPANY IDENTIFICATION

Product name : Caffeine

Product Number : C0750  
Brand : Sigma-Aldrich

Supplier : Sigma-Aldrich  
3050 Spruce Street  
SAINT LOUIS MO 63103  
USA

Telephone : +1 800-325-5832  
Fax : +1 800-325-5052  
Emergency Phone # (For both supplier and manufacturer) : (314) 776-6555

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

### 2. HAZARDS IDENTIFICATION

#### Emergency Overview

##### OSHA Hazards

Target Organ Effect, Toxic by ingestion

##### Target Organs

Central nervous system, HeartCentral nervous system, Heart

##### GHS Classification

Acute toxicity, Oral (Category 4)

##### GHS Label elements, including precautionary statements

Pictogram



Signal word

Warning

Hazard statement(s)

H302

Harmful if swallowed.

Precautionary statement(s)

none

#### HMIS Classification

Health hazard: 2

Chronic Health Hazard: \*

Flammability: 0

Physical hazards: 0

#### NFPA Rating

Health hazard: 2

Fire: 0

Reactivity Hazard: 0

#### Potential Health Effects

##### Inhalation

May be harmful if inhaled. May cause respiratory tract irritation.

**Skin** May be harmful if absorbed through skin. May cause skin irritation.  
**Eyes** May cause eye irritation.  
**Ingestion** Toxic if swallowed.

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### 3. COMPOSITION/INFORMATION ON INGREDIENTS

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

Component		Concentration
<b>Caffeine</b>		
CAS-No.	58-08-2	90 100 %
EC-No.	200-362-1	
Index-No.	613-086-00-5	

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### 4. 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.

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### 5. FIREFIGHTING MEASURES

#### Conditions of flammability

Not flammable or combustible.

#### Suitable extinguishing media

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

#### Special protective equipment for firefighters

Wear self contained breathing apparatus for fire fighting if necessary.

#### Hazardous combustion products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, nitrogen oxides (NO<sub>x</sub>)

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### 6. ACCIDENTAL RELEASE MEASURES

#### Personal precautions

Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Avoid breathing dust.

#### Environmental precautions

Do not let product enter drains.

#### 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.

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### 7. HANDLING AND STORAGE

#### 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.

### Conditions for safe storage

Keep container tightly closed in a dry and well-ventilated place.

Keep in a dry place.

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## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Contains no substances with occupational exposure limit values.

### Personal protective equipment

#### 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).

#### Hand 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: Dermatrill® (KCL 740 / Aldrich Z677272, Size M)

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: Dermatrill® (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.

#### Eye 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 and 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.

#### Hygiene measures

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

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## 9. PHYSICAL AND CHEMICAL PROPERTIES

### Appearance

Form powder

Colour white

### Safety data

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

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

Boiling point no data available

Flash point no data available

Ignition temperature	540 °C (1,004 °F)
Auto-ignition temperature	no data available
Lower explosion limit	no data available
Upper explosion limit	no data available
Vapour pressure	20 hPa (15 mmHg) at 89 °C (192 °F)
Density	1.230 g/cm <sup>3</sup> at 18 °C (64 °F)
Water solubility	18.7 g/l at 16 °C (61 °F)
Partition coefficient: n-octanol/water	log Pow: -0.091 at 23 °C (73 °F)
Relative vapour density	no data available
Odour	odourless
Odour Threshold	no data available
Evaporation rate	no data available

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## 10. STABILITY AND REACTIVITY

### Chemical stability

Stable under recommended storage conditions.

### Possibility of hazardous reactions

no data available

### Conditions to avoid

no data available

### Materials to avoid

Strong oxidizing agents

### Hazardous decomposition products

Other decomposition products - no data available

Hazardous decomposition products formed under fire conditions. - Carbon oxides, nitrogen oxides (NO<sub>x</sub>)

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## 11. TOXICOLOGICAL INFORMATION

### Acute toxicity

#### Oral LD<sub>50</sub>

LD<sub>50</sub> Oral - rat - male and female - 367.7 mg/kg

#### Inhalation LC<sub>50</sub>

LC<sub>50</sub> Inhalation - rat - male and female - 4.94 mg/l

#### Dermal LD<sub>50</sub>

LD<sub>50</sub> Dermal - rat - male and female - > 2,000 mg/kg

#### Other information on acute toxicity

no data available

### Skin corrosion/irritation

Skin - rabbit - No skin irritation - OECD Test Guideline 404

### Serious eye damage/eye irritation

Eyes - rabbit - No eye irritation - OECD Test Guideline 405

### Respiratory or skin sensitisation

mouse - Did not cause sensitisation on laboratory animals.

### Germ cell mutagenicity

Genotoxicity in vitro - rat - Kidney

Micronucleus test

Genotoxicity in vivo - mouse - Oral  
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

### **Teratogenicity**

no data available

### **Specific target organ toxicity - single exposure (Globally Harmonized System)**

no data available

### **Specific target organ toxicity - repeated exposure (Globally Harmonized System)**

no data available

### **Aspiration hazard**

no data available

### **Potential health effects**

<b>Inhalation</b>	May be harmful if inhaled. May cause respiratory tract irritation.
<b>Ingestion</b>	Toxic if swallowed.
<b>Skin</b>	May be harmful if absorbed through skin. May cause skin irritation.
<b>Eyes</b>	May cause eye irritation.

### **Signs and Symptoms of Exposure**

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

### **Synergistic effects**

no data available

### **Additional Information**

RTECS: EV6475000

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## **12. ECOLOGICAL INFORMATION**

### **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 Method: DIN 38412
Toxicity to algae	static test - Desmodesmus subspicatus (green algae) - > 100 mg/l - 72 h Method: OECD Test Guideline 201

### **Persistence and degradability**

no data available

### **Bioaccumulative potential**

no data available

### **Mobility in soil**

no data available

**PBT and vPvB assessment**

no data available

**Other adverse effects**

no data available

**13. DISPOSAL CONSIDERATIONS****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.

**14. TRANSPORT INFORMATION****DOT (US)**

UN number: 1544 Class: 6.1 Packing group: III  
 Proper shipping name: Alkaloids, solid, n.o.s. (Caffeine)  
 Reportable Quantity (RQ):  
 Marine pollutant: No  
 Poison Inhalation Hazard: No

**IMDG**

UN number: 1544 Class: 6.1 Packing group: III EMS-No: F-A, S-A  
 Proper shipping name: ALKALOIDS, SOLID, N.O.S. (Caffeine)  
 Marine pollutant: No

**IATA**

UN number: 1544 Class: 6.1 Packing group: III  
 Proper shipping name: Alkaloids, solid, n.o.s. (Caffeine)

**15. REGULATORY INFORMATION****OSHA Hazards**

Target Organ Effect, Toxic by ingestion

**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****Further information**

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