

## SECTION 1: CHEMICAL PRODUCT and COMPANY IDENTIFICATION

Product Name: Caffeine 99%

Product Code: C00690

Supplier: Pfaltz & Bauer, Inc.  
172 E. Aurora Street  
Waterbury, CT 06708 USA

Phone: 203-574-0075

FAX: 203-574-3181

Emergency Phone: INFOTRAC, US: 1-800-535-5053  
INFOTRAC, INTERNATIONAL: +1-352-323-3500

## SECTION 2: HAZARDS IDENTIFICATION

Statement of Hazard: Environmentally hazardous, Irritant, Respiratory irritant, Toxic

Acute Health Hazard: Irritant to eyes, skin, mucous membranes and respiratory system.  
May be toxic by ingestion, harmful by skin absorption and inhalation.

Chronic Health Hazard: Not Available

HMIS Rating: H: 2 F: 0 P: 0

NFPA Rating: H: 2 F: 0 R: 0

To the best of our knowledge, the toxicological properties of this chemical have not been thoroughly investigated. Use appropriate procedures and precautions to prevent or minimize exposure.

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS):  
GHS Classification in accordance with Regulation (EC) No 1272/2008:

Acute toxicity, dermal (Category 4), H312  
Acute toxicity, inhalation (Category 4), H332  
Acute toxicity, oral (Category 3), H301  
Hazardous to the aquatic environment, acute toxicity (Category 3), H402  
Serious eye damage/eye irritation (Category 2A), H319  
Skin corrosion/irritation (Category 2), H315  
Specific target organ toxicity, single exposure; Respiratory tract irritation (Category 3), H335

Pictogram:



Signal Word:

Warning

Hazard Statement(s):

H301 Toxic if swallowed.  
H312 Harmful in contact with skin.  
H315 Causes skin irritation.  
H319 Causes serious eye irritation.  
H332 Harmful if inhaled.  
H335 May cause respiratory irritation.  
H402 Harmful to aquatic life.

Precautionary Statement(s):

P261 Avoid breathing dust/fume/gas/mist/vapors/spray.  
P264 Wash skin thoroughly after handling.  
P270 Do not eat, drink, or smoke when using this product.  
P273 Avoid release to the environment.  
P280 Wear protective gloves/protective clothing/eye protection/face protection.  
P301+P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.  
P302+P352 IF ON SKIN: wash with plenty of soap and water.  
P304+P340 IF INHALED: Remove victim to fresh air and Keep at rest in a position comfortable for breathing.  
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.  
P332+P313 IF SKIN irritation occurs: Get medical advice/attention.

### **SECTION 3: COMPOSITION/INFORMATION on INGREDIENTS**

Chemical Name:

Caffeine 99%

Synonyms:

1,3,7-Trimethylxanthine; Coffeine; Guanine; Methyltheobromine;  
1,3,7-Trimethyl-2,6-dioxopurine; 1,3,7-Trimethylxanthine

CAS Number:

58-08-2

MDL Number:

MFCD00005758

EINECS Number:

200-362-1

Beilstein Registry Number:

17705

Molecular Formula:

C<sub>8</sub>H<sub>10</sub>N<sub>4</sub>O<sub>2</sub>

Molecular Weight:

194.19

Content:

As specified in product name.

## **SECTION 4: FIRST AID MEASURES**

|                      |  |
|----------------------|--|
| <u>Eye Contact:</u>  | Flush eyes with large amounts of water for fifteen minutes. Separate eyelids with fingers. If irritation persists, seek medical attention. |
| <u>Skin Contact:</u> | Wash skin with soap and water. If irritation persists, seek medical attention.   |
| <u>Ingestion:</u>    | Do not induce vomiting. Seek medical attention.  |
| <u>Inhalation:</u>   | Move to a fresh air environment. Contact a physician if breathing becomes difficult.   |

## **SECTION 5: FIRE FIGHTING MEASURES**

|  |   |
|--|---|
| <u>Flash Point (°C):</u>               | 206   |
| <u>Explosion Limits:</u>               | Not Available   |
| <u>Auto Ignition Temperature (°C):</u> | 540   |
| <u>Extinguishing Media:</u>            | Carbon dioxide, dry chemical powder, alcohol-resistant foam, or water spray |
| <u>Protective Equipment:</u>           | Wear self-contained respirator and fully protective impervious suit.        |
| <u>Specific Hazards:</u>               | May emit hazardous fumes under fire conditions.                             |

## **SECTION 6: ACCIDENTAL RELEASE MEASURES**

|                                  |   |
|----------------------------------|---|
| <u>Personal Protection:</u>      | Wear a self-contained breathing apparatus, rubber boots and gloves, and disposable coveralls. Dispose of coveralls after use. Remove from ignition sources if safe to do so. Follow emergency response plan and contact proper authorities if needed.<br>Keep unprotected persons away. |
| <u>Environmental Protection:</u> | Keep spills out of sewers and bodies of water. Dike and contain the spill with inert material. Absorb on sand, vermiculite or diatomite. Transfer material to a container for disposal or recovery. Ventilate area and wash spill site after material pickup is complete.               |

## **SECTION 7: HANDLING and STORAGE**

|                              |  |
|------------------------------|--|
| <u>Handling and Storage:</u> | Avoid breathing dust, vapor, mist or gas. Avoid contact with skin and eyes. Avoid prolonged or repeated exposure. Use only in a chemical fume hood. Open and handle container with care. Keep ignition sources away.<br>Store in a tightly closed container in a dry, well-ventilated place. |
|------------------------------|--|

Sensitivities: Not Available

Storage Temperature (°C): 15 to 30

## **SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION**

Engineering Controls: Use product in a well ventilated area or under a fume hood. Use proper lab equipment while handling this product. Keep away from incompatible materials for possible risk of hazardous reaction.

Eye Protection: Wear appropriate protective eyeglass or chemical safety goggles. Make sure that there is an eyewash station in your vicinity.

Skin Protection: Wear impervious gloves and protective clothing.

Respiratory Protection: Use a NIOSH approved respirator when exposure limits are exceeded or if irritation or other symptoms are experienced.

| <u>Exposure Limits:</u> | <u>Country</u> | <u>Source</u> | <u>Type</u> | <u>Value</u>  |
|-------------------------|----------------|---------------|-------------|---------------|
|                         | USA            | ACGIH         | TWA         | Not Available |
|                         | USA            | OSHA          | STEL        | Not Available |
|                         | USA            | OSHA          | PEL         | Not Available |

## **SECTION 9: PHYSICAL and CHEMICAL PROPERTIES**

Appearance: White crystalline powder

Odor: Odorless

Odor Threshold: Not Available

Flash Point (°C): 206

Auto Ignition Temperature (°C): 540

UEL % by Volume: Not Available

LEL % by Volume: Not Available

Melting Point (°C): 234-236

Boiling Point (°C): 416.78

Evaporation Rate: Not Available

|   |                                   |
|---|-----------------------------------|
| <u>pH Value:</u>                                      | 5.5 - 6.5 at 10 g/l               |
| <u>Density (g/cm<sup>3</sup>):</u>                    | 1.45                              |
| <u>Refractive Index (n<sup>20</sup><sub>D</sub>):</u> | Not Available                     |
| <u>Viscosity:</u>                                     | Not Available                     |
| <u>Solubility in Water:</u>                           | Soluble, 18.7 g/L at 16 C         |
| <u>Solubility in Other:</u>                           | Soluble in Pyrrole, Ethyl acetate |
| <u>Vapor Pressure (mmHg):</u>                         | Not Available                     |
| <u>Vapor Density (Air=1):</u>                         | Not Available                     |

## **SECTION 10: STABILITY and REACTIVITY**

|  |  |
|--|--|
| <u>Stability:</u>                        | Stable under normal temperatures and pressures.                                      |
| <u>Incompatibility:</u>                  | Strong oxidizing agents  |
| <u>Reactivity:</u>                       | Product may react with incompatible materials to release other hazardous substances. |
| <u>Conditions to Avoid:</u>              | Heat, flame, sparks, other ignition sources.   |
| <u>Hazardous Decomposition Products:</u> | Carbon oxides, Nitrogen oxides   |

## **SECTION 11: TOXICOLOGICAL INFORMATION**

|   |  |                                  |        |                                    |        |   |        |   |        |  |        |
|---|--|----------------------------------|--------|------------------------------------|--------|---|--------|---|--------|--|--------|
| <u>RTECS Reference:</u>                     | EV6475000  |                                  |        |                                    |        |   |        |   |        |  |        |
| <u>Target Organs:</u>                       | Not Available  |                                  |        |                                    |        |   |        |   |        |  |        |
| <u>Toxicity Data:</u>                       | <table> <tr> <td>Oral Rat LD<sub>50</sub> mg/kg:</td> <td>192.00</td> </tr> <tr> <td>Oral Mouse LD<sub>50</sub> mg/kg:</td> <td>168.00</td> </tr> <tr> <td>Intraperitoneal Rat LD<sub>50</sub> mg/kg:</td> <td>240.00</td> </tr> <tr> <td>Intravenous Rat LD<sub>50</sub> mg/kg:</td> <td>105.00</td> </tr> <tr> <td>Subcutaneous Rat LD<sub>50</sub> mg/kg:</td> <td>170.00</td> </tr> </table> | Oral Rat LD <sub>50</sub> mg/kg: | 192.00 | Oral Mouse LD <sub>50</sub> mg/kg: | 168.00 | Intraperitoneal Rat LD <sub>50</sub> mg/kg: | 240.00 | Intravenous Rat LD <sub>50</sub> mg/kg: | 105.00 | Subcutaneous Rat LD <sub>50</sub> mg/kg: | 170.00 |
| Oral Rat LD <sub>50</sub> mg/kg:            | 192.00   |                                  |        |                                    |        |   |        |   |        |  |        |
| Oral Mouse LD <sub>50</sub> mg/kg:          | 168.00   |                                  |        |                                    |        |   |        |   |        |  |        |
| Intraperitoneal Rat LD <sub>50</sub> mg/kg: | 240.00   |                                  |        |                                    |        |   |        |   |        |  |        |
| Intravenous Rat LD <sub>50</sub> mg/kg:     | 105.00   |                                  |        |                                    |        |   |        |   |        |  |        |
| Subcutaneous Rat LD <sub>50</sub> mg/kg:    | 170.00   |                                  |        |                                    |        |   |        |   |        |  |        |
| <u>Carcinogenicity:</u>                     | <p>National Toxicology Program (NTP) listed:<br/>Not Available</p> <p>International Agency for Research on Cancer (IARC) listed: Not Available</p>   |                                  |        |                                    |        |   |        |   |        |  |        |

Potential Symptoms:

Not Available

## SECTION 12: ECOLOGICAL INFORMATION

Toxicity:

Water flea LC<sub>50</sub>:

182.00 mg/l - 182.00 hrs.

## SECTION 13: DISPOSAL CONSIDERATIONS

Contact a licensed professional waste disposal service. Dispose in a manner consistent with federal, state and local environmental regulations.

## SECTION 14: TRANSPORT INFORMATION

DOT Shipping Name: Alkaloids, Solid, N.O.S.

DOT UN Number: UN1544

DOT Hazard Class: Class 6.1

DOT Packing Group: PGIII

IMDG Shipping Name: Alkaloids, Solid, N.O.S.

IMDG UN Number: UN1544

IMDG Hazard Class: Class 6.1

IMDG Packing Group: PGIII

Marine Pollutant: No

IATA Shipping Name: Alkaloids, Solid, N.O.S.

IATA UN Number: UN1544

IATA Hazard Class: Class 6.1

IATA Packing Group: PGIII

## SECTION 15: REGULATORY INFORMATION

United States

Toxic Substance Control Act (TSCA) listed: Yes

Superfund Amendments and Reauthorization Act (SARA 302) listed: No

Superfund Amendments and Reauthorization Act (SARA 311/312) listed: No

Superfund Amendments and Reauthorization Act (SARA 313) listed: No

#### European Union

European Inventory of Existing Chemical Substances (EINECS): 200-362-1

GHS Classification in accordance with Regulation (EC) No 1272/2008: Yes

#### Canada

Canadian Domestic Substances List (DSL) listed: Yes

Canadian Non-Domestic Substances List (NDSL) listed: No

### **SECTION 16: OTHER INFORMATION**

Date Prepared: 9/26/2022

The information above is presented in good faith. It is believed to be accurate and represents the best information currently available to us. However, we make no warranty with respect to such information and we assume no liability resulting from its use. The user should consider this information as a supplement to other information that may be available and make independent judgement to ensure proper use to protect the health and safety of employees and the environment. Pfaltz and Bauer shall not be held liable for any damage resulting from handling or from contact with the above product.