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

Catalogue Number	CS-SR-00045-500GM
Product Name	Caffeine anhydrous pure, 98%
CAS No.	58-08-2
Category	Biochemicals
Synonyms	1,3,7,Trimethylxanthine; 1,3,7-Trimethyl-7H-purine-2,6-dione; 7-Methyltheophylline; 1,3,7-Trimethyl-2,6-dioxopurine; Asia migrine
Brand	Clearsynth Labs Ltd.
Identified uses	Laboratory Chemicals
Uses advised against	Not available
Company	Clearsynth Labs Ltd. Mumbai, India
Emergency Phone #	+91-22-245045900
REACH No.	Not available

SECTION 2: Hazards identification

Disclaimer: This is sample MSDS. Please email **sales@clearsynth.com** for more details.

2.1 Classification of the substance or mixture-Regulation (EC) No 1272/2008:

Acute toxicity (Category 4)

2.2 Label Elements

Signal Word: Warning

Hazard Statement(s)

Code	Statement
H302	Harmful if swallowed.
H301	Not available
H332	Harmful if inhaled.

H360	Not available

Precautionary Statement(s)

Code	Statement
P264	Wash hands thoroughly after handling.
P270	Not available
P301+P317	Not available
P330	Not available
P501	Dispose of contents/container in accordance with local/regional/national/international regulatio
P203	Not available
P261	Avoid breathing dust/fume/gas/mist/vapours/spray.
P271	Use only outdoors or in a well-ventilated area.
P280	Wear protective gloves/protective clothing/eye protection/face protection.
P301+P316	Not available
P304+P340	IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P317	Not available
P318	Not available
P321	Specific treatment (see … on this label).
P405	Store locked up.

SECTION 3: Composition / information on ingredients

3.1 Substance

Component : Caffeine anhydrous pure, 98%
CAS Number : 58-08-2
Molecular Formula : C8H10N4O2
Molecular Weight : 194.19
Parent Chemical : Caffeine
Synonyms : 1,3,7,Trimethylxanthine; 1,3,7-Trimethyl-7H-purine-2,6-dione; 7-Methyltheophylline; 1,3,7-Trimethyl-2,6-dioxopurine; Asia migrine
Concentration : Not available

SECTION 4: First aid measures

SECTION 4: First-aid measures

4.1 Description of first aid measures

General advice: Remove from exposure. Show this SDS to the physician in attendance.
Inhalation: Move person to fresh air. If breathing is difficult, seek medical attention.
Skin contact: Wash with plenty of soap and water. Remove contaminated clothing and wash before reuse. Get medical attention if irritation persists.
Eye contact: Rinse cautiously with water for several minutes. Remove contact lenses if present and easy to do. Continue rinsing. Seek medical attention if irritation persists.
Ingestion: Rinse mouth. Do not induce vomiting unless directed by medical personnel. Seek medical attention.

4.2 Most important symptoms and effects, both acute and delayed
Not available.

4.3 Indication of any immediate medical attention and special treatment needed
Treat symptomatically. Not available.

SECTION 5: Firefighting measures

SECTION 5: Fire-fighting measures

5.1 Extinguishing media
Suitable extinguishing media: Use extinguishing measures appropriate to local circumstances and the surrounding environment (e.g., water spray, alcohol-resistant foam, dry chemical, carbon dioxide).
Unsuitable extinguishing media: Not available.

5.2 Special hazards arising from the substance or mixture
May form combustible dust concentrations in air. Thermal decomposition may produce irritating and/or toxic fumes. Not available.

5.3 Advice for firefighters
Wear self-contained breathing apparatus (SCBA) and full protective gear. Avoid breathing smoke/fumes. Use water spray to cool unopened containers. Prevent fire-fighting water from entering drains or waterways.

SECTION 6: Accidental release measures

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures
Avoid dust formation. Avoid breathing dust. Use appropriate personal protective equipment.

6.2 Environmental precautions
Avoid release to the environment. Prevent entry into drains, surface waters, or soil.

6.3 Methods and material for containment and cleaning up
Contain spill. Sweep up or vacuum using equipment suitable for dusts; avoid generating airborne dust. Place in a suitable, labeled container for disposal. Clean spill area with water after material pickup where appropriate.

6.4 Reference to other sections
See Section 8 for personal protective equipment and Section 13 for disposal considerations.

SECTION-7: Handling and storage

SECTION 7: Handling and storage

7.1 Precautions for safe handling
Handle in accordance with good industrial hygiene and safety practice. Avoid contact with eyes, skin, and clothing. Avoid breathing dust. Minimize dust generation and accumulation. Use local exhaust ventilation where dust may be generated.

7.2 Conditions for safe storage, including any incompatibilities
Store in a tightly closed container in a cool, dry, well-ventilated place. Protect from moisture. Keep away from incompatible materials. Incompatibilities: Not available.

7.3 Specific end use(s)
Laboratory/research use. Not available.

SECTION 8: Exposure controls / personal protection

SECTION 8: Exposure controls/personal protection

8.1 Control parameters
Occupational exposure limits: Not available.
Biological limit values: Not available.

8.2 Exposure controls
Engineering controls: Provide adequate ventilation. Use local exhaust ventilation to control dust exposure.
Personal protective equipment (PPE):
- Eye/face protection: Safety glasses with side shields or chemical splash goggles.
- Skin protection: Protective gloves. Protective clothing as appropriate.
- Respiratory protection: If ventilation is inadequate or dust is generated, use a suitable particulate respirator in accordance with applicable regulations.
- Hygiene measures: Wash hands after handling. Do not eat, drink, or smoke when using this product. Remove contaminated clothing and wash before reuse.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Test	Result
Appearance	No data available
IR spectrum	No data available
pH	No data available
Solubility	No data available

Property	Value
a) Physical State	No data available
b) Color	No data available

Property	Value
c) Odor	No data available
d) pH	2.7
e) Vapour Pressure	No data available
f) Viscosity	No data available
g) Initial Boiling Point and boiling range	No data available
h) Melting Point / Freezing Point	No data available
i) Auto Ignition Temperature	No data available
j) Flash Point	No data available
k) Explosion Limit, Lower	No data available
l) Explosion Limit, Upper	No data available
m) Decomposition Temperature	No data available
n) Loss on Drying	No data available
o) Relative Density	No data available
p) Solubility (in DMSO)	No data available
q) Oxidizing Properties	No data available

SECTION 10: Stability and reactivity

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
Avoid dust formation. Avoid excessive heat. Avoid moisture. Not available.

10.5 Incompatible materials
Not available.

10.6 Hazardous decomposition products
Not available.

SECTION 11: Toxicological information

11.1 Information on toxicological effects

- Acute toxicity: Signs and Symptoms of Overdose Caffeine consumption is generally regarded as safe. Additive caffeine in most substances does not necessitate FDA approval as long as consumption remains within safe levels stipulated by the statute. A typical dose of caffeine is around 70 to 100 mg per drink. While there is no recommended daily allowance for caffeine, doses of up to 400 mg/d are deemed safe. The exact LD50 for humans varies and largely depends on individual sensitivity to caffeine. However, the estimated LD50 is between 150 and 200 mg/kg. Case reports indicate that doses as low as 57 mg/kg have resulted in fatalities. A toxic dose of caffeine, where significant adverse effects such as tachycardia, arrhythmia, altered mentation, and seizures may occur, is estimated to be around 1.2 g. The estimates of a life-threatening dose of caffeine range from 10 to 14 g. Management of Overdose The treatment for mild ingestions primarily involves supportive care. However, in cases of more severe ingestions, additional interventions may be necessary. Patients may require intubation to protect the airway from vomiting or altered mental status. Benzodiazepines can be administered to abort any seizures that develop. If IV fluid resuscitation fails to address persistent hypotension, patients may need vasopressors. Phenylephrine or norepinephrine is typically the first-line vasopressor, with phenylephrine being preferable due to its α-agonism and reflex bradycardia. Magnesium and β-blockers can combat cardiac arrhythmias secondary to the hyperadrenergic response. The ultra-short-acting β1-selective blocker esmolol has been used successfully in several case reports for this indication. In the case of lethal arrhythmias, patients will require defibrillation and resuscitation according to advanced cardiac life support protocols. Additionally, activated charcoal, intralipid infusion, and hemodialysis can aid in preventing further metabolism and subsequent effects of caffeine overdose. Some degree of caffeine intake is almost universal in modern society and an estimated 90% of adults in the United States consume caffeine daily, the average amount being 200 mg daily. Yet despite its widescale use, there is no evidence that regular consumption of caffeine or coffee has adverse effects on the liver. Indeed, epidemiological studies suggest that regular coffee intake may have modest protective effects against the progression of chronic liver disease and development of liver cancer. In high, toxic doses, caffeine can have severe effects on brain, heart and muscle function but has not been linked to clinically apparent liver injury. In contrast, there have been several reports of liver injury linked to use of caffeine rich energy drinks. These reports have not been very convincing and most were not well documented. In many instances, the hepatic injury resembled acute hepatic necrosis or ischemic hepatitis (Case 1). In other cases, other diagnoses were more likely than liver injury from the energy drinks (Case 2). Furthermore, it remains unclear whether the hepatic effects were caused by caffeine per se or to other components in typical energy drinks, such as vitamins, herbs or other botanical products. In reports of caffeine overdose including cases with autopsies, hepatic injury has been absent or not mentioned. Thus, caffeine is unlikely to cause liver injury, but the various high caffeine energy drinks which are widely used may possibly cause liver injury when used to excess. Likelihood score for caffeine: E (unlikely cause of clinically apparent liver injury). Likelihood score for energy drinks: C[H] (probable rare cause of clinically apparent liver injury when used in high amounts).
- Skin corrosion/irritation: No data available.
- Serious eye damage/eye irritation: No data available.
- Respiratory or skin sensitization: No data available.
- Germ cell mutagenicity: No data available.
- Carcinogenicity: Some degree of caffeine intake is almost universal in modern society and an estimated 90% of adults in the United States consume caffeine daily, the average amount being 200 mg daily. Yet despite its widescale use, there is no evidence that regular consumption of caffeine or coffee has adverse effects on the liver. Indeed, epidemiological studies suggest that regular coffee intake may have modest protective effects against the progression of chronic liver disease and development of liver cancer. In high, toxic doses, caffeine can have severe effects on brain, heart and muscle function but has not been linked to clinically apparent liver injury. In contrast, there have been several reports of liver injury linked to use of caffeine rich energy drinks. These reports have not been very convincing and most were not well documented. In many instances, the hepatic injury resembled acute

hepatic necrosis or ischemic hepatitis (Case 1). In other cases, other diagnoses were more likely than liver injury from the energy drinks (Case 2). Furthermore, it remains unclear whether the hepatic effects were caused by caffeine per se or to other components in typical energy drinks, such as vitamins, herbs or other botanical products. In reports of caffeine overdose including cases with autopsies, hepatic injury has been absent or not mentioned. Thus, caffeine is unlikely to cause liver injury, but the various high caffeine energy drinks which are widely used may possibly cause liver injury when used to excess. Likelihood score for caffeine: E (unlikely cause of clinically apparent liver injury). Likelihood score for energy drinks: C[H] (probable rare cause of clinically apparent liver injury when used in high amounts). Evaluation: There is inadequate evidence for the carcinogenicity in humans of caffeine. There is inadequate evidence for the carcinogenicity in experimental animals of caffeine. Overall evaluation: Caffeine is not classifiable as to its carcinogenicity to humans (Group 3).
- Reproductive toxicity: No data available.
- STOT-single exposure: No data available.
- STOT-repeated exposure: Some degree of caffeine intake is almost universal in modern society and an estimated 90% of adults in the United States consume caffeine daily, the average amount being 200 mg daily. Yet despite its widescale use, there is no evidence that regular consumption of caffeine or coffee has adverse effects on the liver. Indeed, epidemiological studies suggest that regular coffee intake may have modest protective effects against the progression of chronic liver disease and development of liver cancer. In high, toxic doses, caffeine can have severe effects on brain, heart and muscle function but has not been linked to clinically apparent liver injury. In contrast, there have been several reports of liver injury linked to use of caffeine rich energy drinks. These reports have not been very convincing and most were not well documented. In many instances, the hepatic injury resembled acute hepatic necrosis or ischemic hepatitis (Case 1). In other cases, other diagnoses were more likely than liver injury from the energy drinks (Case 2). Furthermore, it remains unclear whether the hepatic effects were caused by caffeine per se or to other components in typical energy drinks, such as vitamins, herbs or other botanical products. In reports of caffeine overdose including cases with autopsies, hepatic injury has been absent or not mentioned. Thus, caffeine is unlikely to cause liver injury, but the various high caffeine energy drinks which are widely used may possibly cause liver injury when used to excess. Likelihood score for caffeine: E (unlikely cause of clinically apparent liver injury). Likelihood score for energy drinks: C[H] (probable rare cause of clinically apparent liver injury when used in high amounts). /LABORATORY ANIMALS: Subchronic or Prechronic Exposure/ In a 90-day oral toxicity study, the test substance was administered in drinking water to groups of Fischer 344 rats ... (groups of 12 animals/sex). Rats were given 188, 375, 750, 1500, and 3000 ppm in the drinking water (ca. 19.7, 42, 85.4, 151, 272 mg/kg bw/day for males and 23, 51, 104, 174, and 287 mg/kg bw/day for females, calculated from weight and water consumption); control groups were given tap water. The body weight gains of all treated groups were decreased. The effect was significant in the highest dose only (reduction of 26%, males, 20%, females). Water consumption was decreased in rats given 3000 ppm, whereas it was increased in the 750 and 375 ppm groups. No marked changes in clinical signs of toxicity were observed up to 1500 ppm. No dose-related changes in clinical chemistry were seen. With one exception (cellular enlargement in salivary gland), no pronounced significant changes in gross morphology or microscopic findings were observed. ... No description of adverse effects /were given/. The effect observed in the salivary gland was described as dose dependent in rats ... . The effects in the salivary gland were considered adaptive. Reversible effects in the salivary glands are a well known pharmacological effect of caffeine (sympathicomimetic). These morphological changes are not considered to be an adverse effect of the substance. Finally, microscopic evaluation of sex organs revealed no significant differences between exposed and control rats. NOAEL rat: 1500 ppm (male 151 mg/kg bw/d; female 174 mg/kg bw/d)
- Aspiration hazard: No data available.

Likely routes of exposure
- Signs and Symptoms of Overdose Caffeine consumption is generally regarded as safe. Additive caffeine in most substances does not necessitate FDA approval as long as consumption remains within safe levels stipulated by the

statute. A typical dose of caffeine is around 70 to 100 mg per drink. While there is no recommended daily allowance for caffeine, doses of up to 400 mg/d are deemed safe. The exact LD50 for humans varies and largely depends on individual sensitivity to caffeine. However, the estimated LD50 is between 150 and 200 mg/kg. Case reports indicate that doses as low as 57 mg/kg have resulted in fatalities. A toxic dose of caffeine, where significant adverse effects such as tachycardia, arrhythmia, altered mentation, and seizures may occur, is estimated to be around 1.2 g. The estimates of a life-threatening dose of caffeine range from 10 to 14 g. Management of Overdose The treatment for mild ingestions primarily involves supportive care. However, in cases of more severe ingestions, additional interventions may be necessary. Patients may require intubation to protect the airway from vomiting or altered mental status. Benzodiazepines can be administered to abort any seizures that develop. If IV fluid resuscitation fails to address persistent hypotension, patients may need vasopressors. Phenylephrine or norepinephrine is typically the first-line vasopressor, with phenylephrine being preferable due to its α-agonism and reflex bradycardia. Magnesium and β-blockers can combat cardiac arrhythmias secondary to the hyperadrenergic response. The ultra-short-acting β1-selective blocker esmolol has been used successfully in several case reports for this indication. In the case of lethal arrhythmias, patients will require defibrillation and resuscitation according to advanced cardiac life support protocols. Additionally, activated charcoal, intralipid infusion, and hemodialysis can aid in preventing further metabolism and subsequent effects of caffeine overdose.

Symptoms related to the physical, chemical and toxicological characteristics
- Signs and Symptoms of Overdose Caffeine consumption is generally regarded as safe. Additive caffeine in most substances does not necessitate FDA approval as long as consumption remains within safe levels stipulated by the statute. A typical dose of caffeine is around 70 to 100 mg per drink. While there is no recommended daily allowance for caffeine, doses of up to 400 mg/d are deemed safe. The exact LD50 for humans varies and largely depends on individual sensitivity to caffeine. However, the estimated LD50 is between 150 and 200 mg/kg. Case reports indicate that doses as low as 57 mg/kg have resulted in fatalities. A toxic dose of caffeine, where significant adverse effects such as tachycardia, arrhythmia, altered mentation, and seizures may occur, is estimated to be around 1.2 g. The estimates of a life-threatening dose of caffeine range from 10 to 14 g. Management of Overdose The treatment for mild ingestions primarily involves supportive care. However, in cases of more severe ingestions, additional interventions may be necessary. Patients may require intubation to protect the airway from vomiting or altered mental status. Benzodiazepines can be administered to abort any seizures that develop. If IV fluid resuscitation fails to address persistent hypotension, patients may need vasopressors. Phenylephrine or norepinephrine is typically the first-line vasopressor, with phenylephrine being preferable due to its α-agonism and reflex bradycardia. Magnesium and β-blockers can combat cardiac arrhythmias secondary to the hyperadrenergic response. The ultra-short-acting β1-selective blocker esmolol has been used successfully in several case reports for this indication. In the case of lethal arrhythmias, patients will require defibrillation and resuscitation according to advanced cardiac life support protocols. Additionally, activated charcoal, intralipid infusion, and hemodialysis can aid in preventing further metabolism and subsequent effects of caffeine overdose.

SECTION 12: Ecological information

SECTION 12: Ecological information

12.1 Toxicity
No data available.

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
Not available.

12.6 Endocrine disrupting properties
No data available.

12.7 Other adverse effects
No data available.

SECTION 13: Disposal considerations

SECTION 13: Disposal considerations

13.1 Waste treatment methods
Dispose of contents/container in accordance with local/regional/national/international regulations. Do not discharge to drains.
Contaminated packaging: Dispose of as unused product or according to local requirements.
Waste codes: Not available.

SECTION 14: Transport information

SECTION 14: Transport information

14.1 UN number
Not available.

14.2 UN proper shipping name
Not available.

14.3 Transport hazard class(es)
Not available.

14.4 Packing group
Not available.

14.5 Environmental hazards
Not available.

14.6 Special precautions for user
Not available.

14.7 Maritime transport in bulk according to IMO instruments
Not available.

SECTION 15: Regulatory information

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

Not available.

15.2 Chemical safety assessment
No data available.

SECTION 16: Other information

SECTION 16: Other information

Product name: Caffeine anhydrous pure, 98%
CAS No.: 58-08-2
Catalog No.: CS-SR-00045-500GM
Synonyms: 1,3,7,Trimethylxanthine; 1,3,7-Trimethyl-7H-purine-2,6-dione; 7-Methyltheophylline; 1,3,7-Trimethyl-2,6-dioxopurine; Asia migrine
Supplier: Clearsynth Labs Ltd., Mumbai, India
Emergency phone: +91-22-245045900

Disclaimer: The information provided is believed to be accurate based on available data; however, no warranty is expressed or implied. Users must determine suitability for their particular purpose and comply with applicable laws and regulations.
Revision date: Not available.
Version: Not available.

DISCLAIMER

This MSDS is system-generated. Please verify and confirm all data, statements, and values with the Support Team before use or distribution.