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

| | |
|---|---|
| **Catalogue Number** | CS-O-00486-5GM |
| **Product Name** | Mettler-Toledo Calibration substance ME 18872, Caffeine |
| **CAS No.** | 58-08-2 |
| **Category** | Intermediate |
| **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.<br>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 : Mettler-Toledo Calibration substance ME 18872, Caffeine
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 medical personnel.
- Inhalation: Move person to fresh air. If symptoms persist, get medical attention.
- Skin contact: Wash with soap and water. Remove contaminated clothing and wash before reuse. Get medical attention if irritation develops or persists.
- Eye contact: Rinse cautiously with water for several minutes. Remove contact lenses if present and easy to do. Continue rinsing. Get medical attention if irritation persists.
- Ingestion: Rinse mouth. Do NOT induce vomiting unless directed by medical personnel. Never give anything by mouth to an unconscious person. Get medical attention if unwell.

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: Water spray, alcohol-resistant foam, dry chemical, carbon dioxide.
- Unsuitable extinguishing media: Not available.

5.2 Special hazards arising from the substance or mixture
- Combustible solid; dust may form explosive mixture with air under certain conditions.
- Hazardous combustion products: Carbon oxides; nitrogen oxides (NOx) (Not available for complete list).

5.3 Advice for firefighters
- Wear self-contained breathing apparatus (SCBA) and full protective gear.
- Use water spray to cool unopened containers.
- Avoid breathing smoke, fumes, or decomposition products.

## SECTION 6: Accidental release measures

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures
- Avoid dust formation and breathing dust.
- Use appropriate personal protective equipment (see Section 8).
- Ensure adequate ventilation.

6.2 Environmental precautions
- Prevent further leakage or spillage if safe to do so.
- Avoid release to the environment. Do not allow to enter drains/surface waters/groundwater.

6.3 Methods and material for containment and cleaning up
- Sweep up or vacuum up spillage and collect in suitable container for disposal.
- Avoid generating dust.
- Clean contaminated area with water and detergent as appropriate.

6.4 Reference to other sections

- See Section 8 for exposure controls/personal protection 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. Avoid dust generation.
- Provide adequate ventilation.

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.
- Incompatibilities: Not available.

7.3 Specific end use(s)
- Laboratory/research use. Not available for additional specific uses.

## 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: Use local exhaust ventilation or general ventilation to minimize dust exposure.
- Personal protective equipment (PPE):
- Eye/face protection: Safety glasses with side shields or chemical splash goggles.
- Skin protection: Protective gloves (material not specified). Protective clothing as appropriate.
- Respiratory protection: If dust or airborne concentrations are generated, use a NIOSH/EN-approved particulate respirator as appropriate.
- Hygiene measures: Wash hands after handling. Do not eat, drink, or smoke when using this product.

## 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 |

| Test | Result |
|---|---|
| Solubility | No data available |

| Property | Value |
|---|---|
| a) Physical State | No data available |
| b) Color | No data available |
| 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
- Not available.

10.2 Chemical stability
- Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions
- Not available.

10.4 Conditions to avoid

- Excess heat.
- Dust generation and accumulation.
- Moisture (if applicable).

10.5 Incompatible materials
- Not available.

10.6 Hazardous decomposition products
- Carbon oxides.
- Nitrogen oxides (NOx).

## 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
- Not available.

12.2 Persistence and degradability
- Not available.

12.3 Bioaccumulative potential
- Not available.

12.4 Mobility in soil
- Not available.

12.5 Results of PBT and vPvB assessment
- Not available.

12.6 Endocrine disrupting properties
- Not available.

12.7 Other adverse effects
- Not 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 code: Not available.

## SECTION 14: Transport information

SECTION 14: Transport information

- UN number: Not available.
- UN proper shipping name: Not available.
- Transport hazard class(es): Not available.
- Packing group: Not available.
- Environmental hazards: Not available.
- Special precautions for user: Not available.
- Transport in bulk according to IMO instruments: Not available.

Note: Transport classification may vary by mode and jurisdiction; verify with current regulations and carrier requirements.

## 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
- Not available.

## SECTION 16: Other information

SECTION 16: Other information

- Product name: Mettler-Toledo Calibration substance ME 18872, Caffeine
- Catalog no.: CS-O-00486-5GM
- CAS no.: 58-08-2
- 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 correct but does not purport to be all-inclusive and shall be used only as a guide. Not available indicates data were not provided or not determined for this SDS excerpt.

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