

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

| | |
|-----------------------------|--|
| Catalogue Number | CS-O-41405 |
| Product Name | Caffeine D6 |
| CAS No. | 104819-85-4 |
| Category | Stable Isotopes |
| Synonyms | 1H-Purine-2,6-dione, 3,7-dihydro-1-methyl-3,7-di(methyl-d3)- |
| 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:

Not available

2.2 Label Elements

Signal Word: Not available

Not available

Hazard Statement(s)

| Code | Statement |
|---------------|---------------|
| Not available | Not available |

Precautionary Statement(s)

| Code | Statement |
|---------------|---------------|
| Not available | Not available |

SECTION 3: Composition / information on ingredients

3.1 Substance

Component : Caffeine D6
CAS Number : 104819-85-4
Molecular Formula : C₈H₄D₆N₄O₂
Molecular Weight : 200.12
Parent Chemical : Caffeine
Synonyms : 1H-Purine-2,6-dione, 3,7-dihydro-1-methyl-3,7-di(methyl-d3)-
Concentration : Not available

SECTION 4: First aid measures

SECTION 4: First-aid measures

4.1 Description of first aid measures

- General advice: Seek medical attention if symptoms persist or if large exposure is suspected. Show this SDS to the physician.
- Inhalation: Move person to fresh air. If breathing is difficult, seek medical attention.
- Skin contact: Wash with soap and water. Remove contaminated clothing and wash before reuse.
- 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. No data 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

- Specific hazards: Not available.
- Hazardous combustion products: Carbon oxides; nitrogen oxides (NO_x). Other decomposition products: Not available.

5.3 Advice for firefighters

- Wear self-contained breathing apparatus (SCBA) and full protective gear.
- Use water spray to cool unopened containers.
- Avoid inhalation of combustion products.

SECTION 6: Accidental release measures

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

- Avoid breathing dust. Avoid contact with skin and eyes.
- 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

- Avoid dust formation.
- Collect spilled material using methods that minimize dust generation (e.g., damp wipe or HEPA-filtered vacuum).
- Place in a suitable, closed container for disposal.

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 formation of dust and aerosols.
- Avoid contact with skin, eyes, and clothing.
- Provide adequate ventilation.

7.2 Conditions for safe storage, including any incompatibilities

- Store in a tightly closed container.
- Store in a cool, dry, well-ventilated place.
- Protect from moisture.
- Incompatible materials: Not available.

7.3 Specific end use(s)

- Laboratory/research use. Other uses: 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: Use local exhaust ventilation or other engineering controls to maintain airborne levels below applicable exposure limits (if established). Provide eyewash station and safety shower.
- Personal protective equipment (PPE):
 - Eye/face protection: Safety glasses with side shields or chemical splash goggles.
 - Skin protection: Protective gloves. Specific glove material and breakthrough time: Not available.
 - Body protection: Lab coat or protective clothing.

- Respiratory protection: If dust or aerosols 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 |
| Solubility | No data available |

| Property | Value |
|--|-------------------|
| a) Physical State | No data available |
| b) Color | No data available |
| c) Odor | No data available |
| d) pH | No data available |
| 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 |

| Property | Value |
|-------------------------|-------------------|
| q) Oxidizing Properties | No data available |

SECTION 10: Stability and reactivity

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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

- Excessive heat. Dust generation. Other conditions: Not available.

10.5 Incompatible materials

- Not available.

10.6 Hazardous decomposition products

- Carbon oxides; nitrogen oxides (NOx). Other decomposition products: Not available.

SECTION 11: Toxicological information

11.1 Information on toxicological effects

- Acute toxicity: No data available.
- 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: No data available.
- Reproductive toxicity: No data available.
- STOT-single exposure: No data available.
- STOT-repeated exposure: No data available.
- Aspiration hazard: No data available.

Likely routes of exposure

- No data available.

Symptoms related to the physical, chemical and toxicological characteristics

- Not available.

SECTION 12: Ecological information

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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.
- Recommended disposal method: Not available.
- Contaminated packaging: Dispose of as unused product unless cleaned and permitted by regulations.

SECTION 14: Transport information

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- 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 carrier and applicable regulations.

SECTION 15: Regulatory information

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

- Regulatory listings (e.g., TSCA/REACH/DSL/ENCS/IECSC, etc.): Not available.
- GHS classification: Not available.

15.2 Chemical safety assessment

- No data available.

SECTION 16: Other information

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- Synonyms: 1H-Purine-2,6-dione, 3,7-dihydro-1-methyl-3,7-di(methyl-d3)-
- Parent chemical: Caffeine
- Supplier: Clearsynth Labs Ltd., Mumbai, India
- Emergency phone: +91-22-245045900

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