

# MATERIAL SAFETY DATA SHEETS

## 1-(3-CHLOROPROPYL)THEOBROMINE

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### 1.IDENTIFICATION

#### 1.1 GHS PRODUCT IDENTIFIER

**Product Name** 1-(3-chloropropyl)theobromine

#### 1.2 OTHER MEANS OF IDENTIFICATION

**Product Name** 1-(3-chloropropyl)theobromine

**Other names** 1-(3-Chloropropyl)-3,7-dihydro-3,7-dimethyl-1H-purine-2,6-dione

#### 1.3 RECOMMENDED USE OF THE CHEMICAL AND RESTRICTIONS ON USE

**Identified uses** Industrial and scientific research uses

**Uses advised against** No data available

#### 1.4 SUPPLIER'S DETAILS

**Company** Cleanchem Laboratories LLP

**Address** Plot No.R-80, 2nd Floor, Prama Instruments,TTC Industrial area, Rabale, Navi Mumbai, Maharashtra- 400 701

**Telephone** 022-27601987

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### 2. HAZARD IDENTIFICATION

#### 2.1 CLASSIFICATION OF THE SUBSTANCE OR MIXTURE

NO DATA AVAILABLE

#### 2.2 GHS LABEL ELEMENTS, INCLUDING PRECAUTIONARY STATEMENTS

**Pictogram(s)** No data available

**Signal word** No data available

**Hazard statement(s)** No data available

**Precautionary statement(s)**

**Prevention** No data available

**Response** No data available

**Storage** No data available

**Disposal** No data available

**Hazard(s) not otherwise** None known

**classified (HNOC)** Pharmaceutical related compound of unknown potency.

**Supplemental information**

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### 3. COMPOSITION/INFORMATION ON INGREDIENTS

#### 3.1 SUBSTANCES

NO DATA AVAILABLE

**MOLECULAR FORMULA:** C<sub>10</sub>H<sub>13</sub>CLN<sub>4</sub>O<sub>2</sub>    **MOLECULAR WEIGHT:** 256.69

| Chemical name                                                          | Common names and synonyms | CAS number |
|------------------------------------------------------------------------|---------------------------|------------|
| <b>1-(3-Chloropropyl)-3,7-dihydro-3,7-dimethyl-1H-purine-2,6-dione</b> | NA                        | 74409-52-2 |

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### 4. FIRST-AID MEASURES

#### 4.1 DESCRIPTION OF NECESSARY FIRST-AID MEASURES

##### General advice

Medical attention is required. Consult a doctor. Show this safety data sheet (SDS) to the doctor in attendance

##### Inhalation

If breathing is difficult, remove to fresh air and keep at rest in a position comfortable for breathing.  
Call a physician if symptoms develop or persist.

##### Following skin contact

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

##### Following eye contact

Rinse with pure water for at least 15 minutes. Consult a doctor.

##### Following ingestion

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person.  
Call a doctor or Poison Control Center immediately.

#### 4.2 MOST IMPORTANT SYMPTOMS/EFFECTS, ACUTE AND DELAYED

may cause physiological effects

#### **4.3 INDICATION OF IMMEDIATE MEDICAL ATTENTION AND SPECIAL TREATMENT NEEDED, IF NECESSARY**

Treat symptomatically

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### **5. FIRE-FIGHTING MEASURES**

#### **5.1 EXTINGUISHING MEDIA**

##### **Suitable extinguishing media**

Water, use dry chemical, carbon dioxide or alcohol-resistant foam.

#### **5.2 SPECIFIC HAZARDS ARISING FROM THE CHEMICAL**

Carbon oxides, Nitrogen oxides, Hydrogen fluoride, Sulphur oxides

#### **5.3 SPECIAL PROTECTIVE ACTIONS FOR FIRE-FIGHTERS**

Wear self-contained breathing apparatus for fire fighting if necessary.

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### **6. ACCIDENTAL RELEASE MEASURES**

#### **6.1 Personal precautions, protective equipment and emergency procedures**

Keep unnecessary personnel away. Wear appropriate personal protective equipment. Avoid Inhalation of dust from the spilled material. Do not touch damaged containers or spilled material Unless wearing appropriate protective clothing. Ensure adequate ventilation.

#### **6.2 ENVIRONMENTAL PRECAUTIONS**

Avoid discharge into drains, water courses or onto the ground.

#### **6.3 METHODS AND MATERIALS FOR CONTAINMENT AND CLEANING UP**

Avoid the generation of dusts during clean-up. Sweep up or vacuum up spillage and collect in Suitable container for disposal. Clean surface thoroughly to remove residual contamination. For Waste disposal

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### **7. HANDLING AND STORAGE**

#### **7.1 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

## **7.2 CONDITIONS FOR SAFE STORAGE, INCLUDING ANY INCOMPATIBILITIES**

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

Keep in a dry place.

Storage conditions: Refrigerator

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## **8. EXPOSURE CONTROLS/PERSONAL PROTECTION**

### **8.1 Control parameters**

#### **Occupational Exposure limit values**

No exposure limits noted for ingredient

### **8.2 Appropriate engineering controls**

A laboratory fume hood or other appropriate form of local exhaust ventilations

### **8.3 Individual protection measures, such as personal protective equipment (PPE)**

#### **Eye/face protection**

Wear tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

#### **Skin protection**

Wear fire/flammable resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

#### **Respiratory protection**

Recommended respirators are NIOSH-approved N100 or CEN-approved FFP3 particulate respirators. These are to be only used as

a backup to local exhaust ventilation or other engineering controls. If the respirator is the only means of protection, a full-face

supplied air respirator must be used

#### **Thermal hazards**

Wear appropriate thermal protective clothing, when necessary

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## **9. PHYSICAL AND CHEMICAL PROPERTIES**

### **Physical state**

### **Colour**

**Odour**

**Melting point/ freezing point**

**Boiling point or initial boiling point and boiling range**

**Flammability**

**Lower and upper explosion limit / flammability limit**

**Flash point** NA

**Auto-ignition temperature** NA

**Decomposition temperature** NA

**pH**

**Kinematic viscosity**

**Solubility**

**Partition coefficient n-octanol/water**

**Vapour pressure** NA

**Density and/or relative density** NA

**Relative vapour density** NA

**Particle characteristics** NA

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## **10. STABILITY AND REACTIVITY**

### **10.1 Reactivity**

The product is stable and non-reactive under normal conditions of use, storage and transport

### **10.2 Chemical stability**

Material is stable under normal conditions

### **10.3 Possibility of hazardous reactions**

No dangerous reaction known under conditions of normal use

### **10.4 Conditions to avoid**

Contact with incompatible materials

### **10.5 Incompatible materials**

Strong oxidizing agents

### **10.6 Hazardous decomposition products**

Irritating and/or toxic fumes or gases. Emits toxic fumes under fire conditions.

## 11. TOXICOLOGICAL INFORMATION

### Acute toxicity

- ORAL LD50: NO DATA AVAILABLE
- INHALATION: NO DATA AVAILABLE
- DERMAL: NO DATA AVAILABLE

### Skin corrosion/irritation

No data available

### Serious eye damage/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

Based on available data, the classification criteria are not met

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## 12. ECOLOGICAL INFORMATION

### 12.1 Ecotoxicity

There are no data on the ecotoxicity of this product.

### 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 Other adverse effects

No data available

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## 13. DISPOSAL CONSIDERATIONS

### 13.1 Disposal methods

#### Product

Product may be burned in an incinerator equipped with afterburner and scrubber. Excess and expired materials are to be offered to a licensed hazardous material disposal company. Ensure that all Federal and Local regulations regarding the disposal and destruction of this material are followed.

**Contaminated packaging** Dispose of as above.

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## 14. TRANSPORT INFORMATION

**14.1 DOT:** Not regulated as dangerous goods

**IATA:** Not regulated as dangerous goods

### 14.2 UN Proper Shipping Name

ADR/RID: No data available

IMDG: No data available

IATA: No data available

### 14.2 UN Proper Shipping Name

ADR/RID: No data available

IMDG: No data available

IATA: No data available

### 14.3 Transport hazard class(es)

ADR/RID: No data available

IMDG: No data available

IATA: No data available

#### 14.4 Packing group, if applicable

ADR/RID: No data available

IMDG: No data available

IATA: No data available

#### 14.5 Environmental hazards

ADR/RID: No

IMDG: No

IATA: No

#### 14.6 Special precautions for user

No data available

#### 14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

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It is the shipper's responsibility to determine the correct transport classification at the time of shipment

#### 15. Regulatory information

##### US federal regulations

This product is not known to be a "Hazardous Chemical" as defined by the OSHA Hazard Communication Standard, 29 CFR 1910.1200.

##### TSCA Section 12(b) Export Notification (40 CFR 707, Subpt. D)

Not regulated.

##### European Union

Not regulated.

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##### OSHA Specifically Regulated Substances (29 CFR 1910.1001-1052)

Not regulated.

#### 16. OTHER INFORMATION

##### Abbreviations and acronyms

- CAS: CHEMICAL ABSTRACTS SERVICE
- IATA: INTERNATIONAL AIR TRANSPORTATION ASSOCIATION
- LD50: LETHAL DOSE 50%

Disclaimer: The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. We as supplier shall not be held liable for any damage resulting from handling or from contact with the above product