1. PRODUCT AND COMPANY IDENTIFICATION

Product name : Theobromine
Product Number : T4500
Brand : Sigma
Company : Sigma-Aldrich
            3050 Spruce Street
            SAINT LOUIS MO  63103
            USA
Telephone : +18003255832
Fax : +18003255052
Emergency Phone # : (314) 776-6555

2. COMPOSITION/INFORMATION ON INGREDIENTS

Synonyms : 2,6-Dihydroxy-3,7-dimethylpurine
            3,7-Dimethylxanthine

Formula : C\textsubscript{7}H\textsubscript{8}N\textsubscript{4}O\textsubscript{2}
Molecular Weight : 180.16 g/mol

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<thead>
<tr>
<th>CAS-No.</th>
<th>EC-No.</th>
<th>Index-No.</th>
<th>Concentration</th>
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<td>Theobromine</td>
<td>83-67-0</td>
<td>201-494-2</td>
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3. HAZARDS IDENTIFICATION

Emergency Overview

OSHA Hazards
Target Organ Effect, Harmful by ingestion.

Target Organs
Male reproductive system., Kidney

HMIS Classification

Health Hazard: 1
Chronic Health Hazard: *
Flammability: 0
Physical hazards: 0

NFPA Rating

Health Hazard: 1
Fire: 0
Reactivity Hazard: 0
Potential Health Effects

Inhalation  May be harmful if inhaled. May cause respiratory tract irritation.
Skin       May be harmful if absorbed through skin. May cause skin irritation.
Eyes       May cause eye irritation.
Ingestion  Harmful if swallowed.

4. FIRST AID MEASURES

General advice
Consult a physician. Show this safety data sheet to the doctor in attendance.

If inhaled
If breathed in, move person into fresh air. If not breathing give artificial respiration Consult a physician.

In case of skin contact
Wash off with soap and plenty of water. Consult a physician.

In case of eye contact
Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed
Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

5. FIRE-FIGHTING MEASURES

Flammable properties
Flash point no data available
Ignition temperature no data available

Suitable extinguishing media
Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

Special protective equipment for fire-fighters
Wear self contained breathing apparatus for fire fighting if necessary.

6. ACCIDENTAL RELEASE MEASURES

Personal precautions
Use personal protective equipment. Avoid dust formation. Avoid breathing dust. Ensure adequate ventilation.

Environmental precautions
Do not let product enter drains.

Methods for cleaning up
Pick up and arrange disposal without creating dust. Keep in suitable, closed containers for disposal.

7. HANDLING AND STORAGE

Handling
Avoid formation of dust and aerosols.
Provide appropriate exhaust ventilation at places where dust is formed. Normal measures for preventive fire protection.

Storage
Keep container tightly closed in a dry and well-ventilated place.
Store under inert gas. Air sensitive.
8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Contains no substances with occupational exposure limit values.

Personal protective equipment

Respiratory protection
Where risk assessment shows air-purifying respirators are appropriate use a dust mask type N95 (US) or type P1 (EN 143) respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Hand protection
Handle with gloves. For prolonged or repeated contact use protective gloves.

Eye protection
Safety glasses

Skin and body protection
Choose body protection according to the amount and concentration of the dangerous substance at the work place.

Hygiene measures
Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance
Form solid
Colour white

Safety data
pH no data available
Melting point 345 - 350 °C (653 - 662 °F)
Boiling point no data available
Flash point no data available
Ignition temperature no data available
Lower explosion limit no data available
Upper explosion limit no data available
Water solubility no data available

10. STABILITY AND REACTIVITY

Storage stability
Stable under recommended storage conditions.

Materials to avoid
Strong oxidizing agents

Hazardous decomposition products
Hazardous decomposition products formed under fire conditions. - Carbon oxides, nitrogen oxides (NOx)

11. TOXICOLOGICAL INFORMATION
Acute toxicity
LD50 Oral - rat - 1,265 mg/kg

Irritation and corrosion
no data available

Sensitisation
no data available

Chronic exposure
This product is or contains a component that is not classifiable as to its carcinogenicity based on its IARC, ACGIH, NTP, or EPA classification.

IARC: Group 3 - Not classifiable as to carcinogenicity to humans (Theobromine)
ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.
NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.
OSHA: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

Signs and Symptoms of Exposure
Nausea, Anorexia.

Potential Health Effects

Inhalation May be harmful if inhaled. May cause respiratory tract irritation.
Skin May be harmful if absorbed through skin. May cause skin irritation.
Eyes May cause eye irritation.
Ingestion Harmful if swallowed.
Target Organs Male reproductive system, Kidney.

Additional Information
RTECS: XH2275000

12. ECOLOGICAL INFORMATION
Elimination information (persistence and degradability)
no data available

Ecotoxicity effects
no data available

Further information on ecology
no data available

13. DISPOSAL CONSIDERATIONS
Product
Observe all federal, state, and local environmental regulations.

Contaminated packaging
Dispose of as unused product.

14. TRANSPORT INFORMATION
15. REGULATORY INFORMATION

OSHA Hazards
Target Organ Effect, Harmful by ingestion.

DSL Status
All components of this product are on the Canadian DSL list.

SARA 302 Components
SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components
SARA 313: This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards
Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components
No components are subject to the Massachusetts Right to Know Act.

Pennsylvania Right To Know Components

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New Jersey Right To Know Components

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California Prop. 65 Components
This product does not contain any chemicals known to State of California to cause cancer, birth, or any other reproductive defects.

16. OTHER INFORMATION

Further information
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