

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
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2. COMPOSITION/INFORMATION ON INGREDIENTS

Synonyms : 2,6-Dihydroxy-3,7-dimethylpurine
3,7-Dimethylxanthine
Formula : C₇H₈N₄O₂
Molecular Weight : 180.16 g/mol

CAS-No.	EC-No.	Index-No.	Concentration
Theobromine			
83-67-0	201-494-2	-	-

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

DOT (US)

Not dangerous goods

IMDG

Not dangerous goods

IATA

Not dangerous goods

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

	CAS-No.	Revision Date
Theobromine	83-67-0	

New Jersey Right To Know Components

	CAS-No.	Revision Date
Theobromine	83-67-0	

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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