



Cambridge Isotope Laboratories, Inc.
50 Frontage Road
Andover, MA 01810

Number:
Issue Date

CLM-6154
04/15/11

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MATERIAL SAFETY DATA SHEET

1 CHEMICAL PRODUCT AND COMPANY INFORMATION

Product Description THEOPHYLLINE (DIMETHYL-13C2, 99%)

Cambridge Isotope Laboratories, Inc.
50 Frontage Rd
ANDOVER, MA 01810
USA

E-mail cilsales@isotope.com
Web Site www.isotope.com

Phone Numbers

Emergency Contact Chemtrec
Emergency Phone 1-800-424-9300 (24 hours)

Customer Service 1-800-322-1174 (8:30-5:30 EST)
Phone
Transportation 1-202-483-7616 (24 hours)

2 HAZARDS IDENTIFICATION

OSHA Hazards

Target Organ Effect, Toxic by ingestion, Reproductive hazards, Mutagen

Target Organs

Nerves, Heat Kidney, Smooth muscle

GHS Classification

Acute toxicity, Oral (Category 3)

GHS Label Information

Signal Word Danger

Hazards Identification

Skull & crossbones

Hazard Statement(s)

Toxic if swallowed.
Harmful to aquatic life.

Precautionary Statement(s)

IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.



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HMIS Ratings

Chronic Health	*
Physical	0
Flammability	0
Health	2

NFPA Codes

Fire	0
Health	2
Reactivity	0

Potential Health Effects

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

3 COMPOSITION / INFORMATION ON INGREDIENTS

Composition / Information on Ingredients

Synonyms	1,3-Dimethylxanthine
Chemical Formula	*C ₂ C ₅ H ₈ N ₄ O ₂
Molecular Weight	182.15
CAS No.	58-55-9 (unlabeled)
EC No.	200-385-7

4 FIRST AID MEASURES

First Aid Measures

Eyes	Flush eye with water for 15 minutes. Get medical attention.
Ingestion	Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.
Inhalation	If breathed in, move person to fresh air. If not breathing, give artificial respiration. Consult a physician.
Skin	Wash with soap and plenty of water. Consult a physician.
Additional Information	Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.



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5 FIRE FIGHTING MEASURE

Fire Fighting Measures

Extinguishing Media Use water spray, alcohol-resistant foam, dry chemical, or carbon dioxide.

Fire Fighting Equipment Wear self contained breathing apparatus for fire fighting if necessary.

6 ACCIDENTAL RELEASE MEASURES

Accidental Release Measures

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

Environmental Precautions Do not empty into drains.

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

7 HANDLING AND STORAGE

Precautions for Safe Handling

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

Conditions for Safe Storage

Storage Store at room temperature away from light and moisture.

8 EXPOSURE CONTROL / PERSONAL PROTECTION

Personal Protection

Eyes - Face Wear safety glasses with side shields (or goggles) and a face shield.

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



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Respiratory	When appropriate, use NIOSH/CEN approved respirator.
Protective Clothing	Wear suitable protective clothing and gloves.
Work Hygienic Practices	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

Physical and Chemical Properties (Unlabeled Compound)

Form	Powder
Color	White
Odor	Odourless
pH	No data available
Melting Point	274 - 275 °C (525 - 527 °F)
Boiling Point	No data available
Flashpoint	No data available
Lower Explosion Limit	No data available
Upper Explosion Limit	No data available
Solubility in Water	No data available
Partition Coefficient	log Pow: - 0.02
Auto Ignition Temperature	No data available

10 STABILITY AND REACTIVITY

Stability and Reactivity

Chemical Stability	Stable if stored under recommended conditions.
Conditions to Avoid	Not available
Hazardous decomposition products	Formed under fire conditions: Carbon oxides, nitrogen oxides (NO _x)
Materials to avoid	Strong oxidizing agents



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11 TOXICOLOGICAL INFORMATION

Acute Toxicity

LD50 Oral Rat 225 mg/kg
Serious No data available
Damage/Eye
Irritation

Skin No data available
Corrosion/Irritation

Inhalation No data available

Respiratory or Skin Not available
Sensitization

Germ Cell Laboratory experiments have shown mutagenic effects.
Mutagenicity

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

IARC 3 - Group 3: not classifiable as to its carcinogenicity to humans.

ACGIH No component of this product present at levels greater than or equal to 0.1% is identifiable 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 identifiable 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.

Reproductive Overexposure may cause reproductive disorder(s) based on tests with laboratory animals.
Toxicity

Specific Target Organ Toxicity

Single Exposure No data available
Repeated Exposure No data available

Signs and Symptoms of Exposure

Nausea
Vomiting
Headache
Diarrhea
Epigastric pain
Circulatory collapse



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Other Information

RTECS XH3850000

12 ECOLOGICAL INFORMATION

Toxicity

Toxicity to Fish LC50	Leuciscus idus (Golden orfe) - 100 mg/l - 96 h
Toxicity to Daphnia and Other Aquatic Invertebrates EC50	Daphnia magna (Water flea) - 178 mg/l - 48 h
Toxicity to Algae and Other Aquatic Plants ErC50	Desmodesmus subspicatus (green algae) - > 100 mg/l - 72 h
Persistence and Degradability	Biodegradability: Biotic/Aerobic Result: > 90 - 100 % - Readily biodegradable.
Bioaccumulative Potential	Not available
Mobility in Soil	Not available
PBT and vPvB Assessment	Not available
Other Adverse Effects	Not available

13 DISPOSAL CONSIDERATIONS

Disposal Considerations

Product Disposal Waste materials should be disposed of under conditions which meet Federal, State, and Local environmental control regulations.

14 TRANSPORT INFORMATION

Transportation Information-DOT/IATA/IMDG

UN Number	2811
Prop. Ship. Name	Toxic solids, organic, n.o.s., (Theophylline 13C2)
Hazard Class	6.1



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Packing Group	III
Marine Pollutant	No
Poison Inhalation Hazard	No

15 REGULATORY INFORMATION

Regulatory Information

Target Organ Effect, Toxic by ingestion, Reproductive hazards, Mutagen

SARA

Sara 302 Component No chemicals in this material are subject to the reporting requirements.

Sara 313 Component No chemicals in this material are subject to the reporting requirements.

SARA 311/312 Hazards

Acute (Y/N) Y

Chronic (Y/N) Y

STATE REGULATIONS

Massachusetts Right to Know No

Pennsylvania Right to Know Yes

New Jersey Right to Know Yes

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

Canada

DSL Status All components are on the Canadian DSL list.

EU

Hazard Harmful

Safety Statements

Wear suitable protective clothing.

Risk Statements

Harmful if swallowed.



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16 OTHER INFORMATION

Additional MSDS Information This product is not radioactive. The data given for this product are those of the corresponding unlabeled compound, unless specifically indicated otherwise. Health and safety data for labeled compounds are generally not available, but are assumed to be similar or identical to the corresponding unlabeled compound.

Approved On 04/15/11
Version Number 1