

CHEMICAL PRODUCT AND COMPANY INFORMATION

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

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

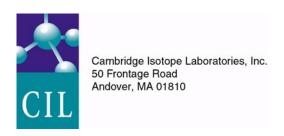
Hazard Statement(s)

Toxic if swallowed.

Harmful to aquatic life.

Precautionary Statement(s)

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



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 *C2C5H8N4O2

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.

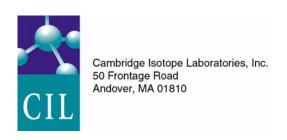
Inhalation If breathed in, move person to fresh air. If not breathing, give artificial respiration. Consult a

physician.

Skin Wash with soap and plenty of water. Consult a physician.

Additional Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of

Information dangerous area.



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 Use personal protective equipment. Avoid dust formation. Avoid breathing dust. Ensure adequate

Precautions ventilation.

Environmental

Precautions

Do not empty into drains.

Methods and Pick up

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.

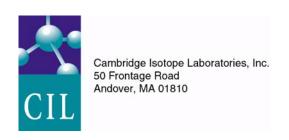
8 EXPOSURE CONTROL / PERSONAL PROTECTION

Personal Protecton

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.



Respiratory When appropriate, use NIOSH/CEN approved respirator.

Protective Clothing Wear suitable protective clothing and gloves.

Work Hygienic Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks

Practices 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 No data available

Limit

Upper Explosion No data available

Limit

Solubility in Water No data available
Partition Coefficient log Pow: - 0.02
Auto Ignition No data available

Temperature

10 STABILITY AND REACTIVITY

Stability and Reactivity

products

Chemical Stability Stable if stored under recommended conditions.

Conditions to Avoid Not available

Hazardous Formed under fire conditions: Carbon oxides, nitrogen oxides (NOx) decomposition

Materials to avoid Strong oxidizing agents

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MATERIAL SAFETY DATA SHEET

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

Sensitization

Not available

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

LABC ACCIL NTB or EBA classification

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

Toxicity

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

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



Other Information

RTECS XH3850000

12 **ECOLOGICAL INFORMATION**

Toxicity

Toxicity to Fish

LC50

Leuciscus idus (Golden orfe) - 100 mg/l - 96 h

Daphnia magna (Water flea) - 178 mg/l - 48 h

Desmodesmus subspicatus (green algae) - > 100 mg/l - 72 h

Toxicity to Daphnia and Other Aquatic

Invertebrates EC50 Toxicity to Algae

and Other Aquatic

Plants ErC50

Persistance and

Biodegradability: Biotic/Aerobic

Degradability 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

DISPOSAL CONSIDERATIONS 13

Disposal Considerations

Waste materials should be disposed of under conditions which meet Federal, State, and Local **Product Disposal**

environmental control regulations.

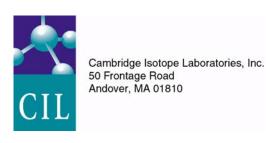
14 TRANSPORT INFORMATION

Transportation Information-DOT/IATA/IMDG

UN Number 2811

Prop. Ship. Name Toxic solids, organic, n.o.s., (Theophylline 13C2)

Hazard Class 6.1



Packing Group
Marine Pollutant

III No

Poison Inhalation

No

Hazard

No

15 REGULATORY INFORMATION

Regulatory Information

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

SARA

Sara 302

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

Component

Sara 313

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

Component

SARA 311/312 Hazards

Acute (Y/N) Y

Chronic (Y/N) Y

STATE REGULATIONS

Massachusetts

No

Right to Know

Pennsylvania Right Yes

to Know

New Jersey Right

Yes

to Know

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.



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 Version Number 04/15/11

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