



# THEOPHYLLINE (2-13C, 99%; 1,3-15N2, 98%+)

## Safety Data Sheet

according to Regulation (EC) No. 453/2010 and according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

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Supersedes: 19/04/2011

Version: 3.0

**CNLM-444**

## SECTION 1: Identification of the substance/mixture and of the company/undertaking

### 1.1. Product identifier

Product form	: Substance
Substance name	: THEOPHYLLINE (2-13C, 99%; 1,3-15N2, 98%+)
EC no	: 200-385-7 (Unlabeled)
CAS No	: 58-55-9 (Unlabeled)
Product code	: CNLM-444
Formula	: C6*CH8N2*N2O2
Synonyms	: 1,3-Dimethylxanthine / 3,7-Dihydro-1,3-dimethyl-1H-purine-2,6-dione / 2,6-Dihydroxy-1,3-dimethylpurine

### 1.2. Relevant identified uses of the substance or mixture and uses advised against

#### 1.2.1. Relevant identified uses

No additional information available

#### 1.2.2. Uses advised against

No additional information available

### 1.3. Details of the supplier of the safety data sheet

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

USA: 1-800-322-1174 Int: 1-978-749-8000  
[cilsales@isotope.com](mailto:cilsales@isotope.com) [www.isotope.com](http://www.isotope.com)

### Emergency telephone number

Emergency numbers:

Chemtrec: 1-800-424-9300 (24 hours)  
International: 1-703-741-5970 (24 hours)

## SECTION 2: Hazards identification

### 2.1. Classification of the substance or mixture

#### Classification according to Regulation (EC) No. 1272/2008 [CLP]

Acute Tox. 3 (Oral) H301

Full text of H-statements: see section 16

#### Classification according to Directive 67/548/EEC [DSD] or 1999/45/EC [DPD]

T; R25

Full text of R-phrases: see section 16

#### GHS-US classification

Acute Tox. 3 (Oral) H301

#### Adverse physicochemical, human health and environmental effects

Nerves, Heat Kidney, Smooth muscle.

### 2.2. Label elements

#### Labelling according to Regulation (EC) No. 1272/2008 [CLP]

Hazard pictograms (CLP)



GHS06

Signal word (CLP)

: Danger

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Hazard statements (CLP)	: H301 - Toxic if swallowed
Precautionary statements (CLP)	: P264 - Wash hands thoroughly after handling P270 - Do not eat, drink or smoke when using this product P301+P310 - IF SWALLOWED: Immediately call a doctor P330 - Rinse mouth P405 - Store locked up P501 - Dispose of contents/container to Comply with applicable regulations

### GHS-US labelling

Hazard pictograms (GHS-US)



GHS06

Signal word (GHS-US)	: Danger
Hazard statements (GHS-US)	: H301 - Toxic if swallowed

Precautionary statements (GHS-US)	: P264 - Wash Both hands thoroughly after handling P270 - Do not eat, drink or smoke when using this product P301+P310 - IF SWALLOWED: immediately call a POISON CENTER or doctor/physician P321 - Specific treatment (see Hazard pictograms (CLP) on this label) P330 - If swallowed, rinse mouth P405 - Store locked up P501 - Dispose of contents/container to Comply with applicable regulations
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### 2.3. Other hazards

No additional information available

## SECTION 3: Composition/information on ingredients

### 3.1. Substance

Name	Product identifier	%	Classification according to Directive 67/548/EEC
THEOPHYLLINE (2-13C, 99%; 1,3-15N2, 98%+) (Main constituent)	(CAS No) 58-55-9 (Unlabeled) (EC no) 200-385-7 (Unlabeled)	100	T; R25
Name	Product identifier	%	Classification according to Regulation (EC) No. 1272/2008 [CLP]
THEOPHYLLINE (2-13C, 99%; 1,3-15N2, 98%+) (Main constituent)	(CAS No) 58-55-9 (Unlabeled) (EC no) 200-385-7 (Unlabeled)	100	Acute Tox. 3 (Oral), H301

Full text of R- and H-statements: see section 16

Name	Product identifier	%	GHS-US classification
THEOPHYLLINE (2-13C, 99%; 1,3-15N2, 98%+) (Main constituent)	(CAS No) 58-55-9 (Unlabeled)	100	Acute Tox. 3 (Oral), H301

Full text of H-statements: see section 16

### 3.2. Mixture

Not applicable

## SECTION 4: First aid measures

### 4.1. Description of first aid measures

First-aid measures general	: Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.
First-aid measures after inhalation	: If breathed in, move person to fresh air. If not breathing, give artificial respiration. Consult a physician.
First-aid measures after skin contact	: Wash with soap and plenty of water. Consult a physician.
First-aid measures after eye contact	: Flush eye with water for 15 minutes. Get medical attention.
First-aid measures after ingestion	: Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

### 4.2. Most important symptoms and effects, both acute and delayed

Symptoms/injuries after inhalation	: May be harmful if inhaled.
Symptoms/injuries after skin contact	: May be harmful if absorbed through skin. May cause skin irritation.

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Symptoms/injuries after eye contact : May cause eye irritation.  
Symptoms/injuries after ingestion : Toxic if swallowed.

### 4.3. Indication of any immediate medical attention and special treatment needed

No additional information available

## SECTION 5: Firefighting measures

### 5.1. Extinguishing media

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

### 5.2. Special hazards arising from the substance or mixture

No additional information available

### 5.3. Advice for firefighters

Firefighting instructions : Wear self contained breathing apparatus for fire fighting if necessary.  
Protection during firefighting : Do not enter fire area without proper protective equipment, including respiratory protection.

## SECTION 6: Accidental release measures

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

#### 6.1.1. For non-emergency personnel

Emergency procedures : Wear respiratory protection. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust.

#### 6.1.2. For emergency responders

No additional information available

### 6.2. Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

### 6.3. Methods and material for containment and cleaning up

For containment : Pick up and arrange disposal without creating dust. Keep in suitable, closed containers for disposal.

### 6.4. Reference to other sections

No additional information available

## SECTION 7: Handling and storage

### 7.1. Precautions for safe handling

Additional hazards when processed : Avoid formation of dust and aerosols. Provide appropriate exhaust ventilation at places where dust is formed. Normal measures for preventive fire protection.

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

### 7.2. Conditions for safe storage, including any incompatibilities

Technical measures : Keep container tightly closed in a dry and well-ventilated place.

Storage conditions : Store at room temperature away from light and moisture.

### 7.3. Specific end use(s)

No additional information available

## SECTION 8: Exposure controls/personal protection

### 8.1. Control parameters

No additional information available

### 8.2. Exposure controls

Personal protective equipment : Gloves. Safety glasses. Protective clothing. Self-contained breathing apparatus.



Hand protection : protective gloves.  
Eye protection : Wear safety glasses with side shields (or goggles) and a face shield.  
Skin and body protection : Choose body protection according to the amount and concentration of the dangerous substance at the work place.  
Respiratory protection : When appropriate, use NIOSH/CEN approved respirator.

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### SECTION 9: Physical and chemical properties

#### 9.1. Information on basic physical and chemical properties

Physical state	: Solid
Appearance	: Powder.
Molecular mass	: 183.14 g/mol (Labeled)
Colour	: White.
Odour	: Odourless.
Odour threshold	: No data available
pH	: No data available
Relative evaporation rate (butylacetate=1)	: No data available
Melting point	: 274 - 275 °C (525 - 527 °F)
Freezing point	: No data available
Boiling point	: No data available
Flash point	: No data available
Auto-ignition temperature	: 610 °C (1,130 °F) at 1,013 hPa (760 mmHg)
Decomposition temperature	: No data available
Flammability (solid, gas)	: No data available
Vapour pressure	: No data available
Relative vapour density at 20 °C	: No data available
Relative density	: 1.36 g/cm <sup>3</sup> at 25 °C (77 °F)
Solubility	: Water: 5.5 g/l at 19.9 °C (67.8 °F)
Log Pow	: -0.007 at 23 °C (73 °F)
Log Kow	: No data available
Viscosity, kinematic	: No data available
Viscosity, dynamic	: No data available
Explosive properties	: No data available
Oxidising properties	: No data available
Explosive limits	: No data available

#### 9.2. Other information

No additional information available

### SECTION 10: Stability and reactivity

#### 10.1. Reactivity

No additional information available

#### 10.2. Chemical stability

Stable if stored under recommended conditions.

#### 10.3. Possibility of hazardous reactions

No additional information available

#### 10.4. Conditions to avoid

Not available.

#### 10.5. Incompatible materials

Strong oxidizing agents.

#### 10.6. Hazardous decomposition products

Formed under fire conditions: Carbon oxides, nitrogen oxides (NO<sub>x</sub>).

### SECTION 11: Toxicological information

#### 11.1. Information on toxicological effects

Acute toxicity : Toxic if swallowed.

THEOPHYLLINE (2-13C, 99%; 1,3-15N2, 98%+) (58-55-9 (Unlabeled))	
LD50 oral rat	272 mg/kg -female
LD50 dermal rat	> 2000 mg/kg - male and female (OECD Test Guideline 402)
LC50 inhalation rat (mg/l)	> 6.7 mg/l/4h - male and female (OECD Test Guideline 403)

Skin corrosion/irritation : Skin - Rabbit Result: No skin irritation. (OECD Test Guideline 404)  
No data available

Serious eye damage/irritation : Eyes - Rabbit Result: No eye irritation. (OECD Test Guideline 405)  
No data available

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Respiratory or skin sensitisation	: Not available No data available
Germ cell mutagenicity	: Mouse - lymphocyte Result: negative. Mouse - male and female. Result: Negative
Carcinogenicity	: This product is or contains a component that is not classifiable as to its carcinogenicity on its IARC, ACGIH, NTP, or EPA classification.
Reproductive toxicity	: Overexposure may cause reproductive disorder(s) based on tests with laboratory animals.
Specific target organ toxicity (single exposure)	: Not classified No data available
Specific target organ toxicity (repeated exposure)	: Not classified No data available
Aspiration hazard	: Not classified
Potential adverse human health effects and symptoms	: Nausea. Vomiting. Headache. Diarrhea. Epigastric pain. Circulatory collapse. To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated. Stomach - Irregularities - Based on Human Evidence.
IARC group	: 3
Symptoms/injuries after inhalation	: May be harmful if inhaled.
Symptoms/injuries after skin contact	: May be harmful if absorbed through skin. May cause skin irritation.
Symptoms/injuries after eye contact	: May cause eye irritation.
Symptoms/injuries after ingestion	: Toxic if swallowed.

## SECTION 12: Ecological information

### 12.1. Toxicity

THEOPHYLLINE (2-13C, 99%; 1,3-15N2, 98%+) (58-55-9 (Unlabeled))	
LC50 fish 1	100 mg/l <i>Leuciscus idus</i> (Golden orfe) - 96 h (DIN 38412)
EC50 Daphnia 1	178 mg/l static test EC50-Daphnia magna (Water flea) - 48 h (Directive 67/548/EEC, Annex V, C.2.)
ErC50 (algae)	> 100 mg/l <i>Desmodesmus subspicatus</i> (green algae) - 72 h (OECD Test Guideline 201)

### 12.2. Persistence and degradability

THEOPHYLLINE (2-13C, 99%; 1,3-15N2, 98%+) (58-55-9 (Unlabeled))	
Persistence and degradability	Result: 90 - 100 % - Readily biodegradable; aerobic - Exposure time 22 d.

### 12.3. Bioaccumulative potential

THEOPHYLLINE (2-13C, 99%; 1,3-15N2, 98%+) (58-55-9 (Unlabeled))	
Log Pow	-0.007 at 23 °C (73 °F)
Bioaccumulative potential	Not available.

### 12.4. Mobility in soil

THEOPHYLLINE (2-13C, 99%; 1,3-15N2, 98%+) (58-55-9 (Unlabeled))	
Ecology - soil	Not available.

### 12.5. Results of PBT and vPvB assessment

No additional information available

### 12.6. Other adverse effects

Other adverse effects : Not available.

## SECTION 13: Disposal considerations

### 13.1. Waste treatment methods

Regional legislation (waste)	: Waste materials should be disposed of under conditions which meet Federal, State, and Local environmental control regulations.
Waste disposal recommendations	: Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.
Ecology - waste materials	: Dispose of as unused product.

## SECTION 14: Transport information

In accordance with ADR / RID / IMDG / IATA / ADN

### 14.1. UN number

UN-No.(DOT)	: 2811
DOT NA no.	UN2811

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### 14.2. UN proper shipping name

Proper Shipping Name (DOT) : Toxic solids, organic, n.o.s.  
Transport hazard class(es) (DOT) : 6.1 - Class 6.1 - Poisonous materials 49 CFR 173.132  
Hazard labels (DOT) : 6.1 - Poison inhalation hazard



DOT Symbols : G - Identifies PSN requiring a technical name  
Packing group (DOT) : III - Minor Danger  
DOT Special Provisions (49 CFR 172.102) : IB8 - Authorized IBCs: Metal (11A, 11B, 11N, 21A, 21B, 21N, 31A, 31B and 31N); Rigid plastics (11H1, 11H2, 21H1, 21H2, 31H1 and 31H2); Composite (11HZ1, 11HZ2, 21HZ1, 21HZ2, 31HZ1 and 31HZ2); Fiberboard (11G); Wooden (11C, 11D and 11F); Flexible (13H1, 13H2, 13H3, 13H4, 13H5, 13L1, 13L2, 13L3, 13L4, 13M1 or 13M2).  
IP3 - Flexible IBCs must be sift-proof and water-resistant or must be fitted with a sift-proof and water-resistant liner.  
T1 - 1.5 178.274(d)(2) Normal..... 178.275(d)(2)  
TP33 - The portable tank instruction assigned for this substance applies for granular and powdered solids and for solids which are filled and discharged at temperatures above their melting point which are cooled and transported as a solid mass. Solid substances transported or offered for transport above their melting point are authorized for transportation in portable tanks conforming to the provisions of portable tank instruction T4 for solid substances of packing group III or T7 for solid substances of packing group II, unless a tank with more stringent requirements for minimum shell thickness, maximum allowable working pressure, pressure-relief devices or bottom outlets are assigned in which case the more stringent tank instruction and special provisions shall apply. Filling limits must be in accordance with portable tank special provision TP3. Solids meeting the definition of an elevated temperature material must be transported in accordance with the applicable requirements of this subchapter.  
DOT Packaging Exceptions (49 CFR 173.xxx) : 153  
DOT Packaging Non Bulk (49 CFR 173.xxx) : 213  
DOT Packaging Bulk (49 CFR 173.xxx) : 240  
Marine pollutant : No

### 14.3. Additional information

Other information : No supplementary information available.

#### Overland transport

Packing group (ADR) : III  
Class (ADR) : 6.1 - Toxic substances  
Hazard identification number (Kemler No.) : 60  
Classification code (ADR) : T2  
Danger labels (ADR) : 6.1 - Toxic substances



Orange plates : An orange rectangular plate with a black border. The number '60' is printed in black in the upper half, and the number '2811' is printed in black in the lower half.

Tunnel restriction code : E  
Limited quantities (ADR) : 5kg  
EAC code : 2X  
Excepted quantities (ADR) : E1

#### Transport by sea

DOT Vessel Stowage Location : A - The material may be stowed "on deck" or "under deck" on a cargo vessel and on a passenger vessel.  
MFAG-No : 154

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### Air transport

DOT Quantity Limitations Passenger aircraft/rail : 100 kg  
(49 CFR 173.27)

DOT Quantity Limitations Cargo aircraft only (49 : 200 kg  
CFR 175.75)

Civil Aeronautics Law : Toxic and infectious substances/Toxic substances(Hazardous materials notice Appended Table  
1 Article 194 of the Enforcement Regulations)

### 14.4. Environmental hazards

Other information : No supplementary information available.

### 14.5. Special precautions for user

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

Not applicable

## SECTION 15: Regulatory information

### 15.1. US Federal regulations

#### THEOPHYLLINE (2-13C, 99%; 1,3-15N2, 98%+) (58-55-9 (Unlabeled))

SARA Section 302 Threshold Planning Quantity (TPQ)	SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.
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SARA Section 313 - Emission Reporting	Not subject to reporting requirements of the United States SARA Section 313;
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### 15.2. International regulations

#### CANADA

#### THEOPHYLLINE (2-13C, 99%; 1,3-15N2, 98%+) (58-55-9 (Unlabeled))

Listed on the Canadian DSL (Domestic Substances List)

#### 15.2.1. National regulations

No additional information available

### 15.3. US State regulations

#### THEOPHYLLINE (2-13C, 99%; 1,3-15N2, 98%+)(58-55-9 (Unlabeled))

State or local regulations	U.S. - New Jersey - Right to Know Hazardous Substance List U.S. - Pennsylvania - RTK (Right to Know) List This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.
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## SECTION 16: Other information

Other 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.

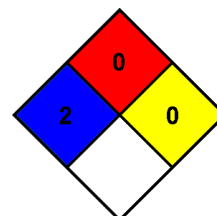
Full text of R-, H- and EUH-statements:

Acute Tox. 3 (Oral)	Acute toxicity (oral), Category 3
H301	Toxic if swallowed
R25	Toxic if swallowed
T	Toxic

NFPA health hazard : 2 - Materials that, under emergency conditions, can cause temporary incapacitation or residual injury.

NFPA fire hazard : 0 - Materials that will not burn under typical dire conditions, including intrinsically noncombustible materials such as concrete, stone, and sand.

NFPA reactivity : 0 - Material that in themselves are normally stable, even under fire conditions.



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### HMIS III Rating

Health	: 2 Moderate Hazard - Temporary or minor injury may occur
Flammability	: 0 Minimal Hazard
Physical	: 0 Minimal Hazard

CIL Multi-Solvent Mixture SDS

*This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product*