



THEOBROMINE (3,7-DIMETHYLXANTHINE) (7-METHYL-D3, 98%)

Safety Data Sheet

according to Regulation (EC) No. 1907/2006 (REACH) with its amendment Regulation (EU) 2015/830 and according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

Date of issue: 29/06/2017

Revision date:

Version: 1.0

DLM-10436

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

1.1. Product identifier

Product form : Substance
Substance name : THEOBROMINE (3,7-DIMETHYLXANTHINE) (7-METHYL-D3, 98%)
EC No : 201-494-2 (Unlabeled)
CAS No : 65566-69-0
Product code : DLM-10436
Formula : C7H5D3N4O2

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

1.2.1. Relevant identified uses

Main use category : Professional use
Industrial/Professional use spec : For professional use only

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 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. 4 (Oral) H302

Full text of hazard classes and H-statements : see section 16

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

Xn; R22

Full text of R-phrases: see section 16

GHS-US classification

Acute Tox. 4 (Oral) H302

Full text of H statements : see section 16

Adverse physicochemical, human health and environmental effects

No additional information available

2.2. Label elements

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

Hazard pictograms (CLP) :



GHS07

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DLM-

10436

Safety Data Sheet

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Signal word (CLP)	: Warning
Hazard statements (CLP)	: H302 - Harmful if swallowed
Precautionary statements (CLP)	: P264 - Wash hands, forearms and face thoroughly after handling P270 - Do not eat, drink or smoke when using this product P301+P312 - IF SWALLOWED: Call a doctor, a POISON CENTER if you feel unwell P330 - Rinse mouth P501 - Dispose of contents/container to hazardous or special waste collection point, in accordance with local, regional, national and/or international regulation

GHS-US labeling

Hazard pictograms (GHS-US)



GHS07

Signal word (GHS-US)	: Warning
Hazard statements (GHS-US)	: H302 - Harmful if swallowed

Precautionary statements (GHS-US)	: P264 - Wash hands, forearms and face thoroughly after handling P270 - Do not eat, drink or smoke when using this product P301+P312 - If swallowed: Call a doctor, a POISON CENTER if you feel unwell P330 - Rinse mouth P501 - Dispose of contents/container to hazardous or special waste collection point, in accordance with local, regional, national and/or international regulation
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2.3. Other hazards

No additional information available

SECTION 3: Composition/Information on ingredients

3.1. Substances

Name	Product identifier	%	Classification according to Directive 67/548/EEC
THEOBROMINE (3,7-DIMETHYLXANTHINE) (7-METHYL-D3, 98%)	(CAS No) 65566-69-0 (EC No) 201-494-2 (Unlabeled) (EC Index No)	100	Xn; R22
Name	Product identifier	%	Classification according to Regulation (EC) No. 1272/2008 [CLP]
THEOBROMINE (3,7-DIMETHYLXANTHINE) (7-METHYL-D3, 98%)	(CAS No) 65566-69-0 (EC No) 201-494-2 (Unlabeled) (EC Index No)	100	Acute Tox. 4 (Oral), H302

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

Name	Product identifier	%	GHS-US classification
THEOBROMINE (3,7-DIMETHYLXANTHINE) (7-METHYL-D3, 98%) (Main constituent)	(CAS No) 65566-69-0	100	Acute Tox. 4 (Oral), H302

Full text of H-phrases: see section 16

3.2. Mixtures

Not applicable

SECTION 4: First aid measures

4.1. Description of first aid measures

First-aid measures general	: If you feel unwell, seek medical advice (show the label where possible). Evacuate danger area.
First-aid measures after inhalation	: When symptoms occur: go into open air and ventilate suspected area. If not breathing, give artificial respiration. Get medical advice/attention.
First-aid measures after skin contact	: Wash with plenty of soap and water. Get immediate medical advice/attention.
First-aid measures after eye contact	: Rinse cautiously with water for several minutes.
First-aid measures after ingestion	: Never give anything by mouth to an unconscious person. Rinse mouth out with water. Get medical advice/attention.

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DLM-

10436

Safety Data Sheet

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

Symptoms/injuries after inhalation	: May be harmful if inhaled. May cause respiratory irritation.
Symptoms/injuries after skin contact	: May be harmful in contact with skin. May cause moderate irritation.
Symptoms/injuries after eye contact	: May cause eye irritation.
Symptoms/injuries after ingestion	: Harmful 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 : Water spray, dry chemical powder, alcohol-resistant foam, carbon dioxide (CO₂).

5.2. Special hazards arising from the substance or mixture

No additional information available

5.3. Advice for firefighters

Firefighting instructions	: Fight fire with normal precautions from a reasonable distance. Wear a self contained breathing apparatus. Do not enter fire area without proper protective equipment, including respiratory protection.
Protection during firefighting	: Do not enter fire area without proper protective equipment, including respiratory protection. Wear recommended personal protective equipment.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

6.1.1. For non-emergency personnel

Emergency procedures : Use personal protective equipment as required. Avoid dust formation. Avoid breathing vapors, mist, gas. Ensure adequate ventilation.

6.1.2. For emergency responders

No additional information available

6.2. Environmental precautions

Prevent entry to sewers and public waters. Do not allow to enter drains or water courses. Avoid release to the environment.

6.3. Methods and material for containment and cleaning up

For containment	: Take up mechanically (sweeping, shoveling) and collect in suitable container for disposal.
Methods for cleaning up	: This material and its container must be disposed of in a safe way, and as per local legislation.

6.4. Reference to other sections

No additional information available

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Precautions for safe handling	: Avoid contact with skin and eyes. Avoid dust formation. Provide adequate ventilation to minimize dust and/or vapor concentrations.
Hygiene measures	: Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work.

7.2. Conditions for safe storage, including any incompatibilities

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

Appropriate engineering controls	: Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work.
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DLM-

10436

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



Materials for protective clothing : Wear suitable protective clothing and gloves.
Hand protection : Wear suitable protective clothing and gloves.
Eye protection : Wear eye protection. Chemical goggles or face shield with safety glasses.
Skin and body protection : Wear suitable protective clothing, gloves and eye/face protection.
Respiratory protection : In case of inadequate ventilation wear respiratory protection. Approved supplied air respirator.
Environmental exposure controls : Avoid release to the environment.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state : Solid
Appearance : Powder.
Molecular mass : 183.18 g/mol (Labeled)
Color : white.
Odor : No data available.
Odor threshold : No data available
pH : No data available
Relative evaporation rate (butyl acetate=1) : No data available
Melting point : 345 °C (653 °F)
Freezing point : No data available
Boiling point : No data available
Flash point : No data available
Auto-ignition temperature : No data available
Decomposition temperature : No data available
Flammability (solid, gas) : No data available
Vapor pressure : No data available
Relative vapor density at 20 °C : No data available
Relative density : No data available
Solubility : No data available
Log Pow : No data available
Log Kow : No data available
Viscosity, kinematic : No data available
Viscosity, dynamic : No data available
Explosive properties : No data available
Oxidizing properties : No data available
Explosion 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

No additional information available

10.5. Incompatible materials

Strong oxidizing agents.

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DLM-

10436

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10.6. Hazardous decomposition products

Carbon oxides (CO, CO₂). Nitrogen oxides.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity : Oral: Harmful if swallowed.

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LD50 oral rat	1265 mg/kg
ATE CLP (oral)	500.000 mg/kg body weight

Skin corrosion/irritation : Not classified

Serious eye damage/irritation : Not classified

Respiratory or skin sensitization : Not classified

Germ cell mutagenicity : Not classified

Carcinogenicity : This is or contains a component that has been reported to be carcinogenic based on its IARC, OSHA, ACGIH, NTP, or EPA classification.

Reproductive toxicity : Not classified

Specific target organ toxicity – single exposure : Not classified

Specific target organ toxicity – repeated exposure : Not classified

Aspiration hazard : Not classified

Potential Adverse human health effects and symptoms : 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. Nausea. Effects on humans. stomach irregularities. Anorexia.

IARC group : 3

Symptoms/injuries after inhalation : May be harmful if inhaled. May cause respiratory irritation.

Symptoms/injuries after skin contact : May be harmful in contact with skin. May cause moderate irritation.

Symptoms/injuries after eye contact : May cause eye irritation.

Symptoms/injuries after ingestion : Harmful if swallowed.

SECTION 12: Ecological information

12.1. Toxicity

Ecology - general : The product is not considered harmful to aquatic organisms or to cause long-term adverse effects in the environment.

12.2. Persistence and degradability

No additional information available

12.3. Bioaccumulative potential

No additional information available

12.4. Mobility in soil

No additional information available

12.5. Results of PBT and vPvB assessment

No additional information available

12.6. Other adverse effects

No additional information 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.

Product/Packaging 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.

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10436

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SECTION 14: Transport information

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

14.1. UN number

Not applicable

14.2. UN proper shipping name

Not applicable

14.3. Additional information

Other information : No supplementary information available.

Special transport precautions : Not classified as dangerous in the meaning of transport regulations.

Overland transport

No additional information available

Transport by sea

No additional information available

Air transport

No additional information available

14.4. Environmental hazards

Other information : No supplementary information available.

14.5. Special precautions for user

Special transport precautions : Not classified as dangerous in the meaning of transport regulations.

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

THEOBROMINE (3,7-DIMETHYLXANTHINE) (7-METHYL-D3, 98%) (65566-69-0)	
SARA Section 302 Threshold Planning Quantity (TPQ)	Not subject to reporting requirements of the United States SARA Section 302.
SARA Section 311/312 Hazard Classes	Immediate (acute) health hazard Delayed (chronic) health hazard
SARA Section 313 - Emission Reporting	Not subject to reporting requirements of the United States SARA Section 313.

15.2. International regulations

CANADA

THEOBROMINE (3,7-DIMETHYLXANTHINE) (7-METHYL-D3, 98%) (65566-69-0)
Listed on the Canadian DSL (Domestic Substances List)

15.2.1. National regulations

No additional information available

15.3. US State regulations

THEOBROMINE (3,7-DIMETHYLXANTHINE) (7-METHYL-D3, 98%)(65566-69-0)	
U.S. - California - Proposition 65 - Carcinogens List	No
U.S. - California - Proposition 65 - Developmental Toxicity	No
U.S. - California - Proposition 65 - Reproductive Toxicity - Female	No
U.S. - California - Proposition 65 - Reproductive Toxicity - Male	No

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DLM-

10436

Safety Data Sheet

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State or local regulations	U.S. - Pennsylvania - RTK (Right to Know) List U.S. - New Jersey - Right to Know Hazardous Substance List
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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.

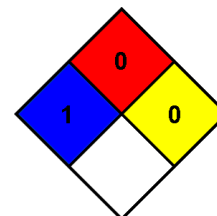
Full text of R-, H- and EUH-phrases:

Acute Tox. 4 (Oral)	Acute toxicity (oral) Category 4
H302	Harmful if swallowed
R22	Harmful if swallowed
Xn	Harmful

NFPA health hazard : 1 - Materials that, under emergency conditions, can cause significant irritation.

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.



HMIS III Rating

Health : 1 Slight Hazard - Irritation or minor reversible injury possible

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