

1. PRODUCT AND COMPANY IDENTIFICATION

Product name : Theophylline

Product Number : T1633
Brand : Sigma

Supplier : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA

Telephone : +1 800-325-5832
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Emergency Phone # (For both supplier and manufacturer) : (314) 776-6555

Preparation Information : Sigma-Aldrich Corporation
Product Safety - Americas Region
1-800-521-8956

2. HAZARDS IDENTIFICATION

Emergency Overview

OSHA Hazards

Target Organ Effect, Toxic by ingestion

Target Organs

Nerves., Heart, Kidney, Smooth muscle.

GHS Classification

Acute toxicity, Oral (Category 3)

GHS Label elements, including precautionary statements

Pictogram



Signal word : Danger

Hazard statement(s)
H301 : Toxic if swallowed.

Precautionary statement(s)
P301 + P310 : IF SWALLOWED: Immediately call a POISON CENTER or doctor/ physician.

HMIS Classification

Health hazard: 2
Chronic Health Hazard: *
Flammability: 0
Physical hazards: 0

NFPA Rating

Health hazard: 2
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 Toxic if swallowed.

3. COMPOSITION/INFORMATION ON INGREDIENTS

Synonyms : 1,3-Dimethylxanthine
3,7-Dihydro-1,3-dimethyl-1H-purine-2,6-dione
2,6-Dihydroxy-1,3-dimethylpurine

Formula : C₇H₈N₄O₂
Molecular Weight : 180.16 g/mol

Component		Concentration
Theophylline		
CAS-No.	58-55-9	90 100 %
EC-No.	200-385-7	

4. FIRST AID MEASURES

General advice

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

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. Take victim immediately to hospital. Consult a physician.

In case of eye contact

Flush eyes with water as a precaution.

If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

5. FIREFIGHTING MEASURES

Conditions of flammability

Not flammable or combustible.

Suitable extinguishing media

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

Special protective equipment for firefighters

Wear self contained breathing apparatus for fire fighting if necessary.

Hazardous combustion products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, nitrogen oxides (NO_x)

6. ACCIDENTAL RELEASE MEASURES

Personal precautions

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

Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

Methods and materials for containment and cleaning up

Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

7. HANDLING AND STORAGE

Precautions for safe handling

Avoid contact with skin and eyes. Avoid formation of dust and aerosols.

Provide appropriate exhaust ventilation at places where dust is formed.

Conditions for safe storage

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

Keep in a dry place.

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 full-face particle respirator type N99 (US) or type P2 (EN 143) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Hand protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: Dermatril® (KCL 740 / Aldrich Z677272, Size M)

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: Dermatril® (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Eye protection

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin and body protection

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Hygiene measures

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance

Form powder

Colour white

Safety data

pH no data available

Melting point/freezing point Melting point/range: 274 - 275 °C (525 - 527 °F)

Boiling point no data available

Flash point	no data available
Ignition temperature	no data available
Auto-ignition temperature	610 °C (1,130 °F) at 1,013 hPa (760 mmHg)
Lower explosion limit	no data available
Upper explosion limit	no data available
Vapour pressure	no data available
Density	1.35 g/cm ³ at 25 °C (77 °F)
Water solubility	5.5 g/l at 19.9 °C (67.8 °F)
Partition coefficient: n-octanol/water	log Pow: -0.007 at 23 °C (73 °F)
Relative vapour density	no data available
Odour	odourless
Odour Threshold	no data available
Evaporation rate	no data available

10. STABILITY AND REACTIVITY

Chemical stability

Stable under recommended storage conditions.

Possibility of hazardous reactions

no data available

Conditions to avoid

no data available

Materials to avoid

Strong oxidizing agents

Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, nitrogen oxides (NO_x)

Other decomposition products - no data available

11. TOXICOLOGICAL INFORMATION

Acute toxicity

Oral LD50

LD50 Oral - rat - female - 272 mg/kg

Inhalation LC50

LC50 Inhalation - rat - male and female - 4 h - > 6.7 mg/l

Dermal LD50

LD50 Dermal - rat - male and female - > 2,000 mg/kg

Other information on acute toxicity

no data available

Skin corrosion/irritation

Skin - rabbit - No skin irritation - OECD Test Guideline 404

Serious eye damage/eye irritation

Eyes - rabbit - No eye irritation - OECD Test Guideline 405

Respiratory or skin sensitisation

no data available

Germ cell mutagenicity

Genotoxicity in vitro - mouse - lymphocyte - with and without metabolic activation - negative

Genotoxicity in vivo - mouse - male and female - Oral - negative

Carcinogenicity

IARC: 3 - Group 3: Not classifiable as to its carcinogenicity to humans (Theophylline)

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.

Reproductive toxicity

no data available

Teratogenicity

no data available

Specific target organ toxicity - single exposure (Globally Harmonized System)

no data available

Specific target organ toxicity - repeated exposure (Globally Harmonized System)

no data available

Aspiration hazard

no data available

Potential health effects

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

Signs and Symptoms of Exposure

Nausea, Vomiting, Headache, Diarrhoea, Epigastric pain., Circulatory collapse

Synergistic effects

no data available

Additional Information

RTECS: XH3850000

12. ECOLOGICAL INFORMATION

Toxicity

Toxicity to fish	LC50 - Leuciscus idus (Golden orfe) - 100 mg/l - 96 h Method: DIN 38412
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 178 mg/l - 48 h Method: Directive 67/548/EEC, Annex V, C.2.
Toxicity to algae	EC50 - Desmodesmus subspicatus (green algae) - > 100 mg/l - 72 h Method: OECD Test Guideline 201

Persistence and degradability

Biodegradability	aerobic Result: 90 - 100 % - Readily biodegradable.
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Bioaccumulative potential

no data available

Mobility in soil

no data available

PBT and vPvB assessment

no data available

Other adverse effects

no data available

13. DISPOSAL CONSIDERATIONS

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

Contaminated packaging

Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)

UN number: 2811 Class: 6.1 Packing group: III
Proper shipping name: Toxic solids, organic, n.o.s. (Theophylline)
Reportable Quantity (RQ):
Marine pollutant: No
Poison Inhalation Hazard: No

IMDG

UN number: 2811 Class: 6.1 Packing group: III EMS-No: F-A, S-A
Proper shipping name: TOXIC SOLID, ORGANIC, N.O.S. (Theophylline)
Marine pollutant: No

IATA

UN number: 2811 Class: 6.1 Packing group: III
Proper shipping name: Toxic solid, organic, n.o.s. (Theophylline)

15. REGULATORY INFORMATION

OSHA Hazards

Target Organ Effect, Toxic by ingestion

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
Theophylline	58-55-9	

New Jersey Right To Know Components

	CAS-No.	Revision Date
Theophylline	58-55-9	

California Prop. 65 Components

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

16. OTHER INFORMATION**Further information**

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