

## MATERIAL SAFETY DATA SHEET

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Version 1.6

## Section 1 - Product and Company Information

Product Name THEOPHYLLINE  
Product Number 88308  
Brand FLUKA

Company Sigma-Aldrich  
Address 3050 Spruce Street  
SAINT LOUIS MO 63103 US

Technical Phone: 800-325-5832  
Fax: 800-325-5052  
Emergency Phone: 314-776-6555

## Section 2 - Composition/Information on Ingredient

Substance Name	CAS #	SARA 313 No
1,3-DIMETHYLBXANTHINE (THEOPHYLLINE)	58-55-9	No

Formula C7H8N4O2

Synonyms Acet-theocin \* Armophylline \* Asmax \* Austyn \*  
3,7-Dihydro-1,3-dimethyl-1H-purine-2,6-dione \*  
1,3-Dimethylxanthine \* Duraphy \* Elixicon \*  
Elixophyllin \* Elixophylline \* Euphyllong \*  
Lanophyllin \* Liguophylline \* NSC 2066 \* Nuelin \*  
Optiphyllin \* Parkophyllin \* Pseudotheophylline \*  
1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-  
(9CI) \* Quibron T/SR \* Slo-Phyllin \* Solosin \*  
Spophyllin retard \* Teofilina (Polish) \*  
Teofyllamin \* Theal tablets \* Theocin \* Theo-Dur  
\* Theofol \* Theograd \* Theolair \* Theolix \*  
Theophyl-225 \* Theophyllin \* Theophylline,  
anhydrous \* Uniphyllin \* Xanthine, 1,3-dimethyl-  
RTECS Number: XH3850000

## Section 3 - Hazards Identification

## EMERGENCY OVERVIEW

Toxic (USA) Harmful (EU).  
Harmful if swallowed.  
Target organ(s): Nerves. Heart.

## HMIS RATING

HEALTH: 2\*  
FLAMMABILITY: 0  
REACTIVITY: 0

## NFPA RATING

HEALTH: 2  
FLAMMABILITY: 0  
REACTIVITY: 0

\*additional chronic hazards present.

For additional information on toxicity, please refer to Section 11.

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#### Section 4 - First Aid Measures

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##### ORAL EXPOSURE

If swallowed, wash out mouth with water provided person is conscious. Call a physician.

##### INHALATION EXPOSURE

If inhaled, remove to fresh air. If not breathing give artificial respiration. If breathing is difficult, give oxygen.

##### DERMAL EXPOSURE

In case of skin contact, flush with copious amounts of water for at least 15 minutes. Remove contaminated clothing and shoes. Call a physician.

##### EYE EXPOSURE

In case of contact with eyes, flush with copious amounts of water for at least 15 minutes. Assure adequate flushing by separating the eyelids with fingers. Call a physician.

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#### Section 5 - Fire Fighting Measures

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##### FLASH POINT

N/A

##### AUTOIGNITION TEMP

N/A

##### FLAMMABILITY

N/A

##### EXTINGUISHING MEDIA

Suitable: Water spray. Carbon dioxide, dry chemical powder, or appropriate foam.

##### FIREFIGHTING

Protective Equipment: Wear self-contained breathing apparatus and protective clothing to prevent contact with skin and eyes.  
Specific Hazard(s): Emits toxic fumes under fire conditions.

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#### Section 6 - Accidental Release Measures

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##### PROCEDURE TO BE FOLLOWED IN CASE OF LEAK OR SPILL

Evacuate area.

##### PROCEDURE(S) OF PERSONAL PRECAUTION(S)

Wear self-contained breathing apparatus, rubber boots, and heavy rubber gloves.

##### METHODS FOR CLEANING UP

Sweep up, place in a bag and hold for waste disposal. Avoid raising dust. Ventilate area and wash spill site after material pickup is complete.

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#### Section 7 - Handling and Storage

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##### HANDLING

User Exposure: Do not breathe dust. Avoid contact with eyes, skin, and clothing. Avoid prolonged or repeated exposure.

STORAGE

Suitable: Keep tightly closed.

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Section 8 - Exposure Controls / PPE

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ENGINEERING CONTROLS

Safety shower and eye bath. Mechanical exhaust required.

PERSONAL PROTECTIVE EQUIPMENT

Respiratory: Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU). Where risk assessment shows air-purifying respirators are appropriate use a dust mask type N95 (US) or type P1 (EN 143) respirator.

Hand: Compatible chemical-resistant gloves.

Eye: Chemical safety goggles.

GENERAL HYGIENE MEASURES

Wash thoroughly after handling.

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Section 9 - Physical/Chemical Properties

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Appearance	Physical State: Solid	
	Color: White	
	Form: Powder	
Property	Value	At Temperature or Pressure
Molecular Weight	180.17 AMU	
pH	N/A	
BP/BP Range	N/A	
MP/MP Range	271 °C	
Freezing Point	N/A	
Vapor Pressure	N/A	
Vapor Density	N/A	
Saturated Vapor Conc.	N/A	
SG/Density	N/A	
Bulk Density	N/A	
Odor Threshold	N/A	
Volatile%	N/A	
VOC Content	N/A	
Water Content	N/A	
Solvent Content	N/A	
Evaporation Rate	N/A	
Viscosity	N/A	
Surface Tension	N/A	
Partition Coefficient	Log Kow: - 0.020	
Decomposition Temp.	N/A	
Flash Point	N/A	
Explosion Limits	N/A	
Flammability	N/A	
Autoignition Temp	N/A	
Refractive Index	N/A	
Optical Rotation	N/A	
Miscellaneous Data	N/A	

N/A = not available

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Section 10 - Stability and Reactivity

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STABILITY

Stable: Stable.

Materials to Avoid: Strong oxidizing agents.

#### HAZARDOUS DECOMPOSITION PRODUCTS

Hazardous Decomposition Products: Carbon monoxide, Carbon dioxide, Nitrogen oxides.

#### HAZARDOUS POLYMERIZATION

Hazardous Polymerization: Will not occur

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### Section 11 - Toxicological Information

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#### ROUTE OF EXPOSURE

Skin Contact: May cause skin irritation.

Skin Absorption: May be harmful if absorbed through the skin.

Eye Contact: May cause eye irritation.

Inhalation: May be harmful if inhaled. Material may be irritating to mucous membranes and upper respiratory tract.

Ingestion: Harmful if swallowed.

#### TARGET ORGAN(S) OR SYSTEM(S)

Nerves. Heart. Smooth muscle. Kidneys.

#### CONDITIONS AGGRAVATED BY EXPOSURE

The toxicological properties have not been thoroughly investigated.

#### TOXICITY DATA

Oral

Woman

130 mg/kg

LDLO

Remarks: Biochemical:Metabolism (intermediary): Other.

Intravenous

Man

3429 UG/KG

LDLO

Remarks: Gastrointestinal:Changes in structure or function of salivary glands. Lungs, Thorax, or Respiration:Cyanosis.

Behavioral:Convulsions or effect on seizure threshold.

Parenteral

Man

12 MG/KG

LDLO

Oral

Rat

225 mg/kg

LD50

Intraperitoneal

Rat

150 MG/KG

LD50

Oral

Mouse

235 mg/kg

LD50

Intraperitoneal

Mouse

70 MG/KG

LD50

Remarks: Behavioral:Convulsions or effect on seizure threshold.

Subcutaneous

Mouse

138 MG/KG

LD50

Intravenous

Mouse

136 MG/KG

LD50

Intramuscular

Mouse

271 MG/KG

LD50

Rectal

Mouse

166 MG/KG

LD50

Remarks: Lungs, Thorax, or Respiration:Other changes.

Behavioral:Muscle contraction or spasticity.

Behavioral:Convulsions or effect on seizure threshold.

Oral

Rabbit

350 mg/kg

LD50

Intravenous

Rabbit

150 MG/KG

LD50

Oral

Guinea pig

183 mg/kg

LD50

#### CHRONIC EXPOSURE - CARCINOGEN

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

#### IARC CARCINOGEN LIST

Rating: Group 3

#### NTP CARCINOGEN LIST

Rating: No evidence.

Species: Mouse/rat

#### CHRONIC EXPOSURE - TERATOGEN

Species: Rat

Dose: 1500 MG/KG

Route of Application: Oral  
Exposure Time: (6-15D PREG)  
Result: Effects on Embryo or Fetus: Fetotoxicity (except death, e.g., stunted fetus).

Species: Rat  
Dose: 1700 MG/KG  
Route of Application: Subcutaneous  
Exposure Time: (1-17D PREG)  
Result: Specific Developmental Abnormalities: Musculoskeletal system.

Species: Mouse  
Dose: 175 MG/KG  
Route of Application: Intraperitoneal  
Exposure Time: (13D PREG)  
Result: Specific Developmental Abnormalities: Craniofacial (including nose and tongue). Specific Developmental Abnormalities: Musculoskeletal system. Specific Developmental Abnormalities: Body wall.

Species: Mouse  
Dose: 200 MG/KG  
Route of Application: Intraperitoneal  
Exposure Time: (13D PREG)  
Result: Effects on Embryo or Fetus: Fetotoxicity (except death, e.g., stunted fetus). Specific Developmental Abnormalities: Other developmental abnormalities.

#### CHRONIC EXPOSURE - MUTAGEN

Result: Laboratory experiments have shown mutagenic effects.

Species: Human  
Dose: 1 MMOL/L  
Cell Type: Other cell types  
Mutation test: Unscheduled DNA synthesis

Species: Human  
Dose: 7 MG/L  
Cell Type: fibroblast  
Mutation test: DNA inhibition

Species: Human  
Dose: 4 MMOL/L  
Cell Type: Other cell types  
Mutation test: DNA inhibition

Species: Human  
Dose: 100 UMOL/L  
Cell Type: lymphocyte  
Mutation test: Other mutation test systems

Species: Human  
Dose: 10 MG/L  
Cell Type: lymphocyte  
Mutation test: Cytogenetic analysis

Species: Human  
Dose: 360 MG/L  
Cell Type: Embryo  
Mutation test: Sister chromatid exchange

Species: Human  
Dose: 10 MG/L  
Cell Type: lymphocyte  
Mutation test: Sister chromatid exchange

Species: Hamster  
Dose: 360 MG/L  
Cell Type: lung  
Mutation test: Sister chromatid exchange

Species: Mouse  
Dose: 6 MMOL/L  
Cell Type: lymphocyte  
Mutation test: DNA inhibition

Species: Mouse  
Dose: 6 MMOL/L  
Cell Type: fibroblast  
Mutation test: DNA inhibition

Species: Rat  
Dose: 1 MMOL/L  
Cell Type: Other cell types  
Mutation test: Other mutation test systems

Species: Mouse  
Dose: 100 UMOL/L  
Cell Type: Other cell types  
Mutation test: Other mutation test systems

Species: Mouse  
Dose: 3200 UMOL/L  
Exposure Time: 24H  
Cell Type: mammary gland  
Mutation test: Cytogenetic analysis

Species: Mouse  
Route: Intraperitoneal  
Dose: 12500 UG/KG  
Mutation test: Sister chromatid exchange

Species: Hamster  
Dose: 6 MMOL/L  
Cell Type: lung  
Mutation test: DNA inhibition

Species: Hamster  
Dose: 450 MG/L  
Cell Type: lung  
Mutation test: Cytogenetic analysis

Species: Hamster  
Dose: 2 MMOL/L  
Cell Type: ovary  
Mutation test: Sister chromatid exchange

Species: Hamster  
Route: Oral  
Dose: 300 MG/KG  
Mutation test: Sister chromatid exchange

Species: Hamster

Dose: 7 MG/L  
Cell Type: lung  
Mutation test: Mutation in mammalian somatic cells.

#### CHRONIC EXPOSURE - REPRODUCTIVE HAZARD

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

Species: Rat  
Dose: 10050 MG/KG  
Route of Application: Oral  
Exposure Time: (67D MALE)  
Result: Paternal Effects: Testes, epididymis, sperm duct.

Species: Rat  
Dose: 75335 MG/KG  
Route of Application: Oral  
Exposure Time: (95D MALE)  
Result: Paternal Effects: Spermatogenesis (including genetic material, sperm morphology, motility, and count).

Species: Mouse  
Dose: 3 GM/KG  
Route of Application: Oral  
Exposure Time: (6-15D PREG)  
Result: Effects on Fertility: Post-implantation mortality (e.g., dead and/or resorbed implants per total number of implants).  
Effects on Embryo or Fetus: Fetotoxicity (except death, e.g., stunted fetus). Effects on Embryo or Fetus: Fetal death.

Species: Mouse  
Dose: 4375 MG/KG  
Route of Application: Oral  
Exposure Time: (7D MALE/7D PRE-3W PREG)  
Result: Effects on Newborn: Live birth index (# fetuses per litter; measured after birth).

Species: Mouse  
Dose: 3720 MG/KG  
Route of Application: Oral  
Exposure Time: (6-15D PREG)  
Result: Effects on Embryo or Fetus: Fetotoxicity (except death, e.g., stunted fetus). Effects on Fertility: Post-implantation mortality (e.g., dead and/or resorbed implants per total number of implants).

Species: Mouse  
Dose: 225 MG/KG  
Route of Application: Intraperitoneal  
Exposure Time: (13D PREG)  
Result: Effects on Fertility: Post-implantation mortality (e.g., dead and/or resorbed implants per total number of implants).

Species: Rabbit  
Dose: 18750 UG/KG  
Route of Application: Intravenous  
Exposure Time: (24-26D PREG)  
Result: Effects on Newborn: Other neonatal measures or effects.

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#### Section 12 - Ecological Information

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#### ACUTE ECOTOXICITY TESTS

Test Type: LC50 Fish  
Species: Leuciscus idus  
Time: 96 h  
Value: 100 mg/l

Test Type: EC50 Daphnia  
Species: Daphnia magna  
Time: 48 h  
Value: 178 mg/l

Test Type: EC50 Algae  
Species: Scenedesmus subspicatus  
Time: 72 h  
Value: > 100 mg/l

#### ELIMINATION

Method: Biotic/Aerobic  
Elimination: > 90.0 - 100.0 %  
Classification: Substantially biodegradable.

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#### Section 13 - Disposal Considerations

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##### APPROPRIATE METHOD OF DISPOSAL OF SUBSTANCE OR PREPARATION

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. Observe all federal, state, and local environmental regulations.

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#### Section 14 - Transport Information

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##### DOT

Proper Shipping Name: Toxic solids, organic, n.o.s.  
UN#: 2811  
Class: 6.1  
Packing Group: Packing Group III  
Hazard Label: Toxic substances.  
PIH: Not PIH

##### IATA

Proper Shipping Name: Toxic solid, organic, n.o.s.  
IATA UN Number: 2811  
Hazard Class: 6.1  
Packing Group: III

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#### Section 15 - Regulatory Information

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##### EU ADDITIONAL CLASSIFICATION

Symbol of Danger: Xn  
Indication of Danger: Harmful.  
R: 22  
Risk Statements: Harmful if swallowed.

##### US CLASSIFICATION AND LABEL TEXT

Indication of Danger: Toxic (USA) Harmful (EU).  
Risk Statements: Harmful if swallowed.  
US Statements: Target organ(s): Nerves. Heart.

##### UNITED STATES REGULATORY INFORMATION

SARA LISTED: No

TSCA INVENTORY ITEM: Yes

CANADA REGULATORY INFORMATION

WHMIS Classification: This product has been classified in accordance with the hazard criteria of the CPR, and the MSDS contains all the information required by the CPR.

DSL: Yes

NDSL: No

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Section 16 - Other Information

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DISCLAIMER

For R&D use only. Not for drug, household or other uses.

WARRANTY

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Inc., shall not be held liable for any damage resulting from handling or from contact with the above product. See reverse side of invoice or packing slip for additional terms and conditions of sale. Copyright 2007 Sigma-Aldrich Co. License granted to make unlimited paper copies for internal use only.