

Revision Date 06-Nov-2010

Revision Number 1

1. PRODUCT AND COMPANY IDENTIFICATION

Product Identifier

Product Description:

Theophylline

Cat No.

250310000; 250310050; 250312500

Synonyms

3,7-Dihydro-1,3-dimethyl-1H-purine-2,6-dione; 1,3-Dimethylxanthine; 1,3-Dimethyl-2,6-dioxo-1,2,3,6-tetrahydropurine

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

Recommended Use

Laboratory chemicals

Uses advised against

No Information available

Details of the supplier of the safety data sheet

Company

Acros Organics BVBA
Janssen Pharmaceuticaaan 3a
2440 Geel, Belgium

E-mail address

begel.sdsdesk@thermofisher.com

Emergency Telephone Number

For information in the US, call: 800-ACROS-01
For information in Europe, call: +32 14 57 52 11

Emergency Number, Europe: +32 14 57 52 99

Emergency Number, US: 201-796-7100

CHEMTREC Phone Number, US: 800-424-9300

CHEMTREC Phone Number, Europe: 703-527-3887

2. HAZARDS IDENTIFICATION

Classification of the substance or mixture

REGULATION (EC) No 1272/2008

Acute oral toxicity

Category 4

Classification according to EU Directives 67/548/EEC or 1999/45/EC

For the full text of the R phrases mentioned in this Section, see Section 16

Symbol(s)

Xn - Harmful

R -phrase(s)

R22 - Harmful if swallowed

Label Elements



2. HAZARDS IDENTIFICATION

Signal Word

Warning

Hazard Statements

H302 - Harmful if swallowed

Precautionary Statements - EU (§28, 1272/2008)

P301+ P312 - IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell

Other Hazards

No information available.

3. COMPOSITION/INFORMATION ON INGREDIENTS

| Component | EC No. | Weight % | CAS-No | Classification | GHSCLAS | REACH Reg. No. |
|--------------|-------------------|----------|---------|----------------|---------------------|----------------|
| Theophylline | EEC No. 200-385-7 | 99 | 58-55-9 | Xn; R22 | Acute Tox. 4 (H302) | |

For the full text of the R phrases mentioned in this Section, see Section 16

4. FIRST AID MEASURES

Description of first aid measures**Eye Contact**

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes Obtain medical attention

Skin Contact

Wash off immediately with soap and plenty of water removing all contaminated clothes and shoes Obtain medical attention

Ingestion

Clean mouth with water Get medical attention

Inhalation

Remove from exposure, lie down Move to fresh air If breathing is difficult, give oxygen If not breathing, give artificial respiration Obtain medical attention

Notes to Physician

Treat symptomatically

5. FIRE-FIGHTING MEASURES

Extinguishing media**Suitable Extinguishing Media**Water spray Carbon dioxide (CO₂) Dry chemical chemical foam**Extinguishing media which must not be used for safety reasons**

No information available.

Special hazards arising from the substance or mixture

Thermal decomposition can lead to release of irritating gases and vapors

Advice for fire-fighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear

6. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures

Ensure adequate ventilation

Environmental precautions

Prevent further leakage or spillage if safe to do so

Methods and material for containment and cleaning up

Sweep up or vacuum up spillage and collect in suitable container for disposal Do not let this chemical enter the environment

7. HANDLING AND STORAGE

Precautions for Safe Handling

Avoid contact with skin and eyes Do not breathe dust Do not breathe vapors or spray mist Do not ingest

Conditions for safe storage, including any incompatibilities

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

Specific End Uses

8. EXPOSURE CONTROLS / PERSONAL PROTECTION

Control parameters

Exposure limits

This product, as supplied, does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies.

Derived No Effect Level (DNEL)

No information available.

Predicted No Effect Concentration (PNEC)

No information available.

Exposure controls

Engineering Measures

Ensure adequate ventilation, especially in confined areas

Personal protective equipment

Eye Protection

Goggles

Hand Protection

Protective gloves

Skin and body protection

Wear appropriate protective gloves and clothing to prevent skin exposure

Respiratory Protection

Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced

Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice

Environmental exposure controls

No information available.

9. PHYSICAL AND CHEMICAL PROPERTIES

Physical State

Powder, Solid

Appearance

White

odor

odorless

pH

5.8 g/l aq.sol.

Boiling Point/Range

No information available.

9. PHYSICAL AND CHEMICAL PROPERTIES

| | |
|----------------------------|-----------------------------|
| Melting Point/Range | 270 - 274°C / 518 - 525.2°F |
| Flash Point | No information available. |
| Water Solubility | 8.3 g/L (20°C) |
| Molecular Formula | C7 H8 N4 O2 |
| Molecular Weight | 180.17 |

10. STABILITY AND REACTIVITY

Reactivity**Chemical Stability**

Stable under normal conditions

Possibility of Hazardous Reactions**Hazardous Polymerization** Hazardous polymerization does not occur.**Hazardous Reactions .** No information available.**Conditions to Avoid**

Incompatible products.

Incompatible Materials

Strong oxidizing agents.

Hazardous Decomposition ProductsNitrogen oxides (NO_x). Carbon monoxide (CO). Carbon dioxide (CO₂).

11. TOXICOLOGICAL INFORMATION

Information on Toxicological Effects**Acute Toxicity****Product Information** No acute toxicity information is available for this product**Component Information****Component**

Theophylline

| | LD50 Oral | LD50 Dermal | LC50 Inhalation |
|--|-------------------|-------------|-----------------|
| | 225 mg/kg (Rat) | | |

Chronic Toxicity**Carcinogenicity**

There are no known carcinogenic chemicals in this product

Sensitization

No information available.

Mutagenic Effects

No information available

Reproductive Effects

No information available.

Developmental Effects

No information available.

Target Organs

No information available.

Other Adverse Effects

The toxicological properties have not been fully investigated. See actual entry in RTECS for complete information

Endocrine Disruptor Information

None known

12. ECOLOGICAL INFORMATION

Toxicity

Ecotoxicity effects Do not empty into drains

Persistence and degradability

No information available

Bioaccumulative potential

No information available.

Mobility in soil

No information available.

Results of PBT and vPvB assessment**Other adverse effects**

No information available

13. DISPOSAL CONSIDERATIONS

Waste treatment methods

Waste from Residues / Unused Products Dispose of in accordance with local regulations

Contaminated Packaging

Empty containers should be taken for local recycling, recovery or waste disposal

14. TRANSPORT INFORMATION

IMDG/IMO

UN-No 2811
Hazard Class 6.1
Packing Group III
Proper Shipping Name TOXIC SOLID, ORGANIC, N.O.S.

ADR

UN-No 2811
Hazard Class 6.1
Packing Group III
Proper Shipping Name TOXIC SOLID, ORGANIC, N.O.S.

IATA

UN-No 2811
Hazard Class 6.1
Packing Group III
Proper Shipping Name TOXIC SOLID, ORGANIC, N.O.S.*

15. REGULATORY INFORMATION

Safety, health and environmental regulations/legislation specific for the substance or mixture**International Inventories**

| Component | EINECS | ELINCS | NLP | TSCA | DSL | NDSL | PICCS | ENCS | CHINA | AICS | KECL |
|-----------|--------|--------|-----|------|-----|------|-------|------|-------|------|------|
| | | | | | | | | | | | |

| | | | | | | | | | | | |
|--------------|---|---|--|---|---|---|---|---|---|---|---------------|
| Theophylline | - | - | | X | X | - | X | X | X | X | KE-10629 X |
|--------------|---|---|--|---|---|---|---|---|---|---|---------------|

Legend

TSCA - United States Toxic Substances Control Act Section 8(b) Inventory

EINECS/ELINCS - European Inventory Lists

DSL/NDSL - Canadian Domestic Substances List/Non-Domestic Substances List

PICCS - Philippines Inventory of Chemicals and Chemical Substances

ENCS - Japan Existing and New Chemical Substances

CHINA - China Inventory of Existing Chemical Substances

AICS - Inventory of Chemical Substances

KECL - Existing and Evaluated Chemical Substances

Chemical Safety Assessment**16. OTHER INFORMATION****Text of R phrases mentioned in Section 2-3**

R22 - Harmful if swallowed

Revision Date 06-Nov-2010

Revision Summary Not applicable

This safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006

Disclaimer

The information provided on this SDS is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guide for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered as a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other material or in any process, unless specified in the text

End of Safety Data Sheet