

1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

1.1 Product identifiers

Product name : Theophylline
CAS-No. : 58-55-9

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

Identified uses : Laboratory chemicals, Manufacture of substances

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008 [EU-GHS/CLP]
Acute toxicity, Oral (Category 3)

Classification according to EU Directives 67/548/EEC or 1999/45/EC
Harmful if swallowed.

2.2 Label elements

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

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.

Supplemental Hazard Statements
none

According to European Directive 67/548/EEC as amended.

Hazard symbol(s)

R-phrases(s)
R22 Harmful if swallowed.

S-phrases(s)
none

2.3 Other hazards - none

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

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

EC-No. 200-385-7

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4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice

Consult a physician. Show this safety data sheet to the doctor in attendance.

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.

4.2 Most important symptoms and effects, both acute and delayed

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

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

no data available

5. FIRE-FIGHTING 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

Carbon oxides, nitrogen oxides (NOx)

5.3 Precautions for fire-fighters

Wear self contained breathing apparatus for fire fighting if necessary.

5.4 Further information

no data available

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and 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.

6.2 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 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.

6.4 Reference to other sections

For disposal see section 13.

7. HANDLING AND STORAGE

7.1 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.Normal measures for preventive fire protection.

7.2 Conditions for safe storage, including any incompatibilities

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

Store under inert gas. Air sensitive.

7.3 Specific end uses

no data available

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters

8.2 Exposure controls

Appropriate engineering controls

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

Personal protective equipment

Eye/face 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 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.

The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

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.

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).

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a) Appearance Form: powder
Colour: white
b) Odour odourless
c) Odour Threshold no data available
d) pH no data available
e) Melting/freezing point Melting point/range: 271 - 273 °C
f) Initial boiling point and boiling range no data available
g) Flash point no data available
h) Evaporation rate no data available
i) Flammability (solid, gas) no data available
j) Upper/lower flammability or explosive limits no data available
k) Vapour pressure no data available
l) Vapour density no data available
m) Relative density no data available
n) Water solubility no data available
o) Partition coefficient: n-octanol/water log Pow: -0,02
p) Autoignition temperature no data available
q) Decomposition temperature no data available
r) Viscosity no data available
s) Explosive properties no data available
t) Oxidizing properties no data available

9.2 Other safety information

no data available

10. STABILITY AND REACTIVITY

10.1 Reactivity

no data available

10.2 Chemical stability

no data available

10.3 Possibility of hazardous reactions

no data available

10.4 Conditions to avoid

no data available

10.5 Incompatible materials

Strong oxidizing agents

10.6 Hazardous decomposition products

Other decomposition products - no data available

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - rat - 225 mg/kg

Skin corrosion/irritation

no data available

Serious eye damage/eye irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

Laboratory experiments have shown mutagenic effects.

Carcinogenicity

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: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

Reproductive toxicity

no data available

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

Specific target organ toxicity - single exposure

no data available

Specific target organ toxicity - repeated exposure

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

Additional Information

RTECS: XH3850000

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to fish LC50 - Leuciscus idus (Golden orfe) - 100 mg/l - 96 h

Toxicity to daphnia and other aquatic invertebrates. EC50 - Daphnia magna (Water flea) - 178 mg/l - 48 h

Toxicity to algae EC50 - Desmodesmus subspicatus (green algae) - > 100 mg/l - 72 h

12.2 Persistence and degradability

Biodegradability Biotic/Aerobic
Result: > 90 - 100 % - Readily biodegradable.

12.3 Bioaccumulative potential

no data available

12.4 Mobility in soil

no data available

12.5 Results of PBT and vPvB assessment

no data available

12.6 Other adverse effects

Harmful to aquatic life.
no data available

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

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

14.1 UN-Number

ADR/RID: 2811 IMDG: 2811 IATA: 2811

14.2 UN proper shipping name

ADR/RID: TOXIC SOLID, ORGANIC, N.O.S. (Theophylline)

IMDG: TOXIC SOLID, ORGANIC, N.O.S. (Theophylline)

IATA: Toxic solid, organic, n.o.s. (Theophylline)

14.3 Transport hazard class(es)

ADR/RID: 6.1 IMDG: 6.1 IATA: 6.1

14.4 Packaging group

ADR/RID: III IMDG: III IATA: III

14.5 Environmental hazards

ADR/RID: no IMDG Marine pollutant: no IATA: no

14.6 Special precautions for users

no data available

15. REGULATORY INFORMATION

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

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

no data available

15.2 Chemical Safety Assessment

no data available

16. OTHER INFORMATION

Further information

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. Lookchem 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.

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