

Safety Data Sheet

according to Regulation (EC) No 1907/2006 (REACH)
Classifications according to Regulation (EC) No 1272/2008.
Printdate 15 May 2023

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

1.1. Product name:

Theophylline

1.1. Catalog No.:

679300

1.2. Relevant identified uses of the substance or mixture

Identified: Laboratory chemical
uses: R&D

1.3. Uses advised against:

HPC Standards GmbH
Am Wieseneck 7

04451 Cunnersdorf
Deutschland

Tel. +49 34291 3372-36
Fax. +49 34291 3372-39
contact@hpc-standards.com

1.4. Emergency telephone number

HPC Standards Tel. +49 34291 3372-36
This number is only available during office hours.

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture
Classification according to Regulation (EC) No 1272/2008
Acute toxicity, Oral (Category 3), H301 Classification according to EU Directives 67/548/EEC or 1999/45/EC
Xn Harmful R22

2.2. Label elements

2.2.1. Pictogram



2.2.2.

2.2 Label elements
Labelling according Regulation (EC) No 1272/2008
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
2.3 Other hazards - none

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances
Formula : C₇H₈N₄O₂
Molecular Weight : 180,16 g/mol
CAS-No. : 58-55-9
EC-No. : 200-385-7
Hazardous ingredients according to Regulation (EC) No 1272/2008
Component Classification Concentration
Theophylline
CAS-No.
EC-No.
58-55-9
200-385-7
Acute Tox. 3; H301 <= 100 %
Hazardous ingredients according to Directive 1999/45/EC
Component Classification Concentration
Theophylline
CAS-No.
EC-No.
58-55-9
200-385-7
Xn, R22 <= 100 %

3.1.1. Formula

C₇H₈N₄O₂

3.1.2. Molecular Weight (g/mol)

180.16

3.1.3. CAS-No.

58-55-9

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

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

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 Advice for firefighters

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

For personal protection see section 8.

6.2 Environmental precautions

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

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.

For precautions see section 2.2.

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. Keep in a dry place.

7.3 Specific end use(s)

A part from the uses mentioned in section 1.2 no other specific uses are stipulated

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 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).

Control of environmental exposure

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

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 point/freezing point

Melting point/range: 274 - 275 °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 1,35 g/cm³ at 25 °C
n) Water solubility 5,5 g/l at 19,9 °C
o) Partition coefficient: noctanol/
water
log Pow: -0,007 at 23 °C
p) Auto-ignition
temperature
610 °C at 1.013 hPa
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
Stable under recommended storage conditions.
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
In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects
Acute toxicity
LD₅₀ Oral - rat - female - 272 mg/kg
LC₅₀ Inhalation - rat - male and female - 4 h - > 6,7 mg/l
(OECD Test Guideline 403)
LD₅₀ Dermal - rat - male and female - > 2.000 mg/kg
(OECD Test Guideline 402)
Skin corrosion/irritation
Skin - rabbit
Result: No skin irritation
(OECD Test Guideline 404)
Serious eye damage/eye irritation
Eyes - rabbit
Result: No eye irritation
(OECD Test Guideline 405)
Respiratory or skin sensitisation
no data available
Germ cell mutagenicity
mouse
lymphocyte
Result: negative
mouse - male and female
Result: negative
Carcinogenicity

IARC: 3 - Group 3: Not classifiable as to its carcinogenicity to humans (Theophylline) Reproductive toxicity
no data available
Specific target organ toxicity - single exposure
no data available
Specific target organ toxicity - repeated exposure
no data available
Aspiration hazard
no data available
Additional Information
RTECS: XH3850000
Nausea, Vomiting, Headache, Diarrhoea, Epigastric pain., Circulatory collapse

12. ECOLOGICAL INFORMATION

12.1 Toxicity
Toxicity to fish LC50 - *Leuciscus idus* (Golden orfe) - 100 mg/l - 96 h
(DIN 38412)
Toxicity to daphnia and
other aquatic
invertebrates
static test EC50 - *Daphnia magna* (Water flea) - 178 mg/l - 48 h
(Directive 67/548/EEC, Annex V, C.2.)
Toxicity to algae EC50 - *Desmodesmus subspicatus* (green algae) - > 100 mg/l - 72 h
(OECD Test Guideline 201)
12.2 Persistence and degradability
Biodegradability aerobic - Exposure time 22 d
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
PBT/vPvB assessment not available as chemical safety assessment not required/not conducted
12.6 Other adverse effects
no data available

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods
Product
Offer surplus and non-recyclable solutions to a licensed disposal company. 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 user
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
For this product a chemical safety assessment was not carried out

16. OTHER INFORMATION

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. For lab use only!