



Safety data sheet

according to 1907/2006/EC, Article 31

Printing date 25.09.2023

version: 1

Revision: 25.09.2023

1.1 Product identifier:

Trade name: **Theobromine**

Article number: 89808

CAS Number:

83-67-0

EC number:

201-494-2

Registration number 01-2120123730-69-0001, 01-2120123730-69-XXXX

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

No further relevant information available.

Application of the substance / the preparation: Reference substance

1.3 Details of the supplier of the safety data sheet:

Manufacturer/Supplier:

PhytoLab GmbH & Co. KG

Dutendorfer Str. 5-7

D-91487 Vestenbergsgreuth

Tel.: Germany/9163/88-327

Fax: Germany/9163/88-456

Mail: ref-substances@phytolab.de

Further information obtainable from: Material Safety Data Sheet: PLV_MSDS@phytolab.com

1.4 Emergency telephone number: Germany/9163/88-500

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture:

Classification according to Regulation (EC) No 1272/2008:



GHS07

Acute Tox. 4 H302 Harmful if swallowed.

Eye Irrit. 2 H319 Causes serious eye irritation.

2.2 Label elements:

Labelling according to Regulation (EC) No 1272/2008:

The substance is classified and labelled according to the CLP regulation.

Hazard pictograms:



GHS07

Signal word: Warning

Hazard statements:

H302 Harmful if swallowed.

H319 Causes serious eye irritation.

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Precautionary statements

- P264 Wash hands thoroughly after handling.
P280 Wear eye protection / face protection.
P301+P312 IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell.
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P337+P313 If eye irritation persists: Get medical advice/attention.
P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

2.3 Other hazards:

Restricted to professional users. The toxicological properties of this compound have not been fully evaluated.

Results of PBT and vPvB assessment:

PBT: Not applicable.

vPvB: Not applicable.

SECTION 3: Composition/information on ingredients**3.1 Substances**

Synonyms: Theobromine

CAS No. Description

83-67-0 Theobromine

Identification number(s)

EC number: 201-494-2

Additional information: chemical product

SECTION 4: First aid measures**4.1 Description of first aid measures:**

General information:

Immediately remove any clothing soiled by the product.

Induce vomiting only with medical help.

After inhalation: Supply fresh air and to be sure call for a doctor.

After skin contact:

Immediately rinse with water.

If skin irritation continues, consult a doctor.

After eye contact:

Rinse opened eye for several minutes under running water. If symptoms persist, consult a doctor.

After swallowing:

Rinse out mouth and then drink plenty of water.

If symptoms persist consult doctor.

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4.2 Most important symptoms and effects, both acute and delayed:

No further relevant information available.

4.3 Indication of any immediate medical attention and special treatment needed:

No further relevant information available.

SECTION 5: Firefighting measures

5.1 Extinguishing media:

Suitable extinguishing agents:

CO₂, powder or water spray. Fight larger fires with water spray or alcohol resistant foam.

Use fire extinguishing methods suitable to surrounding conditions.

5.2 Special hazards arising from the substance or mixture:

No further relevant information available.

5.3 Advice for firefighters:

Protective equipment:

Wear fully protective suit.

Mount respiratory protective device.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures:

Avoid formation of dust.

Wear protective equipment. Keep unprotected persons away.

6.2 Environmental precautions: Do not allow to enter sewers/ surface or ground water.

6.3 Methods and material for containment and cleaning up:

Pick up mechanically.

Dispose contaminated material as waste according to section 13.

6.4 Reference to other sections:

See Section 7 for information on safe handling.

See Section 8 for information on personal protection equipment.

See Section 13 for disposal information.

SECTION 7: Handling and storage

7.1 Precautions for safe handling: Handling corresponding to laboratory safety guidelines.

Information about fire - and explosion protection: No special measures required.

7.2 Conditions for safe storage, including any incompatibilities:

Storage:

Requirements to be met by storerooms and receptacles:

Store in a cool location.

Store only in the original receptacle.

Information about storage in one common storage facility: Store away from foodstuffs.

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Further information about storage conditions:

Store in cool, dry conditions in well sealed receptacles.

Store in the dark.

Recommended storage temperature: 15-25 °C

Storage class: 13

7.3 Specific end use(s): No further relevant information available.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters:

Ingredients with limit values that require monitoring at the workplace: Not required.

Additional information: The lists valid during the making were used as basis.

8.2 Exposure controls:

Appropriate engineering controls: No further data; see section 7.

Individual protection measures, such as personal protective equipment:

General protective and hygienic measures:

The usual precautionary measures are to be adhered to when handling chemicals.

Immediately remove all soiled and contaminated clothing

Avoid contact with the eyes and skin.

Keep away from foodstuffs, beverages and feed.

Wash hands before breaks and at the end of work.

Respiratory protection:

Required in case of dust formation.

Use suitable respiratory protective device in case of insufficient ventilation.

Hand protection:

The glove material has to be impermeable and resistant to the product/ the substance/ the preparation.

Selection of the glove material on consideration of the penetration times, rates of diffusion and the degradation

Material of gloves:



Nitrile rubber, NBR

The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer.

Penetration time of glove material:

The exact break through time has to be found out by the manufacturer of the protective gloves and has to be observed.

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Eye/face protection:



Tightly sealed goggles

Body protection: Protective work clothing

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties:

General Information:

Physical state:	Solid
Colour:	According to Certificate of Analysis
Odour:	No data available.
Odour threshold:	Not determined.
Molecular Weight	
Melting point/freezing point:	351 °C (ECHA)
Boiling point or initial boiling point and boiling range:	Undetermined.
Flammability:	Product is not flammable.
Dust explosion class:	
Lower and upper explosion limit:	
Lower:	Not determined.
Upper:	Not determined.
Flash point:	Not applicable.
(Minimum) Ignition temperature:	Not determined.
Decomposition temperature:	Not determined.
Powder volume resistivity:	
pH:	Not applicable.
Dissociation constant:	
Viscosity:	
Kinematic viscosity:	Not applicable.
Solubility in other solvents:	
Dynamic:	Not applicable.
Solubility:	
water:	sparingly soluble
Partition coefficient n-octanol/water (log value) at 20 °C:	-0.78 (ECHA)
Vapour pressure:	Not applicable.
Density and/or relative density:	
Density at 20 °C:	1.522 g/cm ³ (EU A.3)
Relative density:	Not determined.
Vapour density:	Not applicable.

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Particle characteristics:

See section 3.

9.2 Other information:

Appearance:

Form: Solid

Important information on protection of health and environment, and on safety.

Ignition temperature: Not determined.

Explosive properties: Product does not present an explosion hazard.

Molecular formula C₇ H₈ N₄ O₂

Molecular weight 180.17 g/mol

Oxidising properties: Not determined.

Evaporation rate: Not applicable.

Information with regard to physical hazard classes:

Explosives Void

Flammable gases Void

Aerosols Void

Oxidising gases Void

Gases under pressure Void

Flammable liquids Void

Flammable solids Void

Self-reactive substances and mixtures Void

Pyrophoric liquids Void

Pyrophoric solids Void

Self-heating substances and mixtures Void

Substances and mixtures, which emit flammable gases in contact with water Void

Oxidising liquids Void

Oxidising solids Void

Organic peroxides Void

Corrosive to metals Void

Desensitised explosives Void

SECTION 10: Stability and reactivity

10.1 Reactivity: No further relevant information available.

10.2 Chemical stability:

Thermal decomposition / conditions to be avoided:

Stable under constant-temperature (see 7.)

10.3 Possibility of hazardous reactions: No data available.

10.4 Conditions to avoid: No further relevant information available.

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10.5 Incompatible materials: Strong oxidising agents.

10.6 Hazardous decomposition products: No data available

SECTION 11: Toxicological information

11.1 Information on hazard classes as defined in Regulation (EC) No 1272/2008

Acute toxicity: Harmful if swallowed.

LD/LC50 values relevant for classification:

Oral LD50 837 mg/kg (mouse)

[ECHA]

1,265 mg/kg (rat)

[RTECS/ECHA]

Skin corrosion/irritation: Based on available data, the classification criteria are not met.

Serious eye damage/irritation: Causes serious eye irritation.

Respiratory or skin sensitisation:

Based on available data, the classification criteria are not met.

Germ cell mutagenicity: Based on available data, the classification criteria are not met.

Carcinogenicity: Based on available data, the classification criteria are not met.

Reproductive toxicity: Based on available data, the classification criteria are not met.

STOT-single exposure: Based on available data, the classification criteria are not met.

STOT-repeated exposure: Based on available data, the classification criteria are not met.

Aspiration hazard: Based on available data, the classification criteria are not met.

Additional toxicological information:

The product should be handled with the care usual when dealing with chemicals.

11.2 Information on other hazards

Endocrine disrupting properties: Substance is not listed.

SECTION 12: Ecological information

12.1 Toxicity:

Aquatic toxicity:

Quantitative data concerning the ecological properties of the product are not available.

12.2 Persistence and degradability: No further relevant information available.

12.3 Bioaccumulative potential:

Due to the distribution coefficient n-octanol/water an accumulation in organisms is not expected.

12.4 Mobility in soil: No further relevant information available.

12.5 Results of PBT and vPvB assessment:

PBT: Not applicable.

vPvB: Not applicable.

12.6 Endocrine disrupting properties:

The product does not contain substances with endocrine disrupting properties.

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12.7 Other adverse effects:

Remark: Do not release into sewage, water or soil.

Additional ecological information:

General notes:

Water hazard class 1 (German Regulation) (Assessment by list): slightly hazardous for water

Do not allow undiluted product or large quantities of it to reach ground water, water course or sewage system.

SECTION 13: Disposal considerations**13.1 Waste treatment methods:**

Recommendation:

Dispose product and packaging in accordance with regional environmental laws.

Must not be disposed together with household garbage. Do not allow product to reach sewage system.

Uncleaned packaging:

Recommendation: Disposal must be made according to official regulations.

SECTION 14: Transport information**14.1 UN number or ID number:**

ADR, ADN, IMDG, IATA

Void

14.2 UN proper shipping name:

ADR, ADN, IMDG, IATA

Void

14.3 Transport hazard class(es):

ADR, ADN, IMDG, IATA

Class

Void

14.4 Packing group:

ADR, IMDG, IATA

Void

14.5 Environmental hazards:

Marine pollutant:

No

14.6 Special precautions for user:

Not applicable.

14.7 Maritime transport in bulk according to

IMO instruments:

Not applicable.

UN "Model Regulation":

Void

EU

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SECTION 15: Regulatory information

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

Directive 2012/18/EU:

Named dangerous substances - ANNEX I: Substance is not listed.

DIRECTIVE 2011/65/EU on the restriction of the use of certain hazardous substances in electrical and electronic equipment – Annex II:

Substance is not listed.

REGULATION (EU) 2019/1148

Annex I - RESTRICTED EXPLOSIVES PRECURSORS (Upper limit value for the purpose of licensing under Article 5(3)):

Substance is not listed.

Annex II - REPORTABLE EXPLOSIVES PRECURSORS: Substance is not listed.

National regulations:

Information about limitation of use:

When using chemicals, legal regulations have to be regarded (chemical law, maternity protection, protection of minors).

Waterhazard class: Water hazard class 1 (Assessment by list): slightly hazardous for water.

15.2 Chemical safety assessment: A Chemical Safety Assessment has not been carried out.

SECTION 16: Other information

This information is based on our present knowledge. However, this shall not constitute a guarantee for any specific product features and shall not establish a legally valid contractual relationship.

Abbreviations and acronyms:

RID: Règlement international concernant le transport des marchandises dangereuses par chemin de fer (Regulations Concerning the International Transport of Dangerous Goods by Rail)

IATA-DGR: Dangerous Goods Regulations by the "International Air Transport Association" (IATA)

ICAO: International Civil Aviation Organisation

ICAO-TI: Technical Instructions by the "International Civil Aviation Organisation" (ICAO)

ADR: Accord relatif au transport international des marchandises dangereuses par route (European Agreement Concerning the International Carriage of Dangerous Goods by Road)

IMDG: International Maritime Code for Dangerous Goods

IATA: International Air Transport Association

GHS: Globally Harmonised System of Classification and Labelling of Chemicals

EINECS: European Inventory of Existing Commercial Chemical Substances

CAS: Chemical Abstracts Service (division of the American Chemical Society)

LC50: Lethal concentration, 50 percent

LD50: Lethal dose, 50 percent

PBT: Persistent, Bioaccumulative and Toxic

vPvB: very Persistent and very Bioaccumulative

Acute Tox. 4: Acute toxicity – Category 4

Eye Irrit. 2: Serious eye damage/eye irritation – Category 2