

# SAFETY DATA SHEET

## SECTION 1: Identification of the substance/mixture and of the company/undertaking

### 1.1 Product identifiers

Product Name: 1-(3-Hydroxypropyl)theobromine  
 CAS Number: 59413-14-8  
 Catalog number: A949000

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

Identified uses: All chemicals from Amadis Chemical are for laboratory or manufacturing use only, not for drug, food and household use.

### 1.3 Details of the supplier of the safety data sheet

Amadis Chemical Company Limited  
 Email: [sales@amadischem.com](mailto:sales@amadischem.com)  
 Web: [www.amadischem.com](http://www.amadischem.com)  
 Tel: 0086-571-89925085

### 1.4 Emergency telephone number

Emergency Phone: 0086-571-89925085

## SECTION 2: Hazards identification

### 2.1 Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008  
 No Resource File

### 2.2 GHS Label elements, including precautionary statements

Pictogram  
 Signal word  
 Hazard statement(s)  
 Precautionary statement(s)

### 2.3 Other hazards

None

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Synonyms :  
 Formula : C<sub>10</sub>H<sub>14</sub>N<sub>4</sub>O<sub>3</sub>  
 Molecular weight : g/mol  
 CAS-No. : 59413-14-8

For the full text of the H-Statements mentioned in this Section, see Section 16.

## SECTION 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. Consult a physician.

**In case of eye contact**

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

**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

**SECTION 5: Firefighting 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 (NO<sub>x</sub>), silicon oxides

**5.3 Advice for firefighters**

Wear self-contained breathing apparatus for firefighting if necessary.

**5.4 Further information**

No data available

**SECTION 6: Accidental release measures****6.1 Personal precautions, protective equipment and emergency procedures**

Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation.

Evacuate personnel to safe areas.

For personal protection see section 8.

**6.2 Environmental precautions**

Do not let product enter drains.

**6.3 Methods and materials for containment and cleaning up**

Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

**6.4 Reference to other sections**

For disposal see section 13.

**SECTION 7: Handling and storage****7.1 Precautions for safe handling**

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.

Normal measures for preventive fire protection.

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. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Moisture sensitive. Store under nitrogen.

Storage class (TRGS 510): Combustible liquids not in Storage Class 3

### 7.3 Specific end use(s)

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

## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### 8.2 Exposure controls

##### **Appropriate engineering controls**

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

##### **Personal protective equipment**

##### **Eye/face protection**

Tightly fitting safety goggles. Faceshield (8-inch minimum). 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 (US) or type ABEK (EN14387) respirator cartridges as a backup to engine 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**

Do not let product enter drains.

## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

Appearance

b) Odour No data available

c) Odour Threshold No data available

d) pH No data available

e) Melting point/freezing point

f) Initial boiling point and boiling range

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

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m) Relative density	
o) Partition coefficient: noctanol/water	No data available
p) Auto-ignition 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

## SECTION 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

Acids, Bases, Alcohols, Strong oxidizing agents, Material generates methanol on contact with water or moisture

### 10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NO<sub>x</sub>), silicon oxides

Other decomposition products - No data available

In the event of fire: see section 5

## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

No data available

#### Skin corrosion/irritation

No data available

#### Serious eye damage/eye irritation

No data available

#### Respiratory or skin sensitisation

No data available

#### Germ cell mutagenicity

No data available

#### Carcinogenicity

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

#### Specific target organ toxicity - single exposure

Inhalation - May cause respiratory irritation.

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**Additional Information**

No data available

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Material may form a siloxane polymer on the skin, eyes, or in the lungs. If tissues, seek medical attention.

**SECTION 12: Ecological information**

**12.1 Toxicity**

No data available

**12.2 Persistence and degradability**

No data available

**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**

No data available

**SECTION 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.

**Contaminated packaging**

Dispose of as unused product

**SECTION 14: Transport information**

**14.1 UN number**

ADR/RID:

IMDG:

IATA:

**14.2 UN proper shipping name**

ADR/RID: 1-(3-Hydroxypropyl)theobromine

IMDG: 1-(3-Hydroxypropyl)theobromine

IATA: 1-(3-Hydroxypropyl)theobromine

**14.3 Transport hazard class(es)**

ADR/RID:

IMDG:

IATA:

**14.4 Packaging group**

ADR/RID:

IMDG:

IATA:

**14.5 Environmental hazards**

ADR/RID:

IMDG Marine pollutant:

IATA:

**14.6 Special precautions for user**

No data available

**SECTION 15: Regulatory information****15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture**

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

**15.2 Chemical safety assessment**

For this product a chemical safety assessment was not carried out

**SECTION 16: Other information**

**Full text of H-Statements referred to under sections 2 and 3.**

**Further information**

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