

# MATERIAL SAFETY DATA SHEET

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

### 1.1 Product identifiers

**Product name** : Theobromine  
**Catalogue number** : 0678  
**CAS NUMBER** : 83-67-0 **EC Number** : 201-494-2

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

Reagent for research use only.

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

Z.I Lyon Nord  
Impasse Jacquard - C.S 30062  
69727 GENAY CEDEX - FRANCE  
Phone : (33)(0)478-98-20-34  
Fax : (33)(0)478-98-19-45  
info@extrasynthese.com

### 1.4 Emergency call number (I.N.R.S France) : Tel :

(33)(0)145-42-59-59

## 2 . HAZARDS IDENTIFICATION

### 2.1 Classification of the substance or mixture

According to Regulation (EC) No 1272/2008

Acute oral toxicity (Category 4) ; H302

Carcinogenictiy (Category 2) ; H351

### 2.2 Label elements

Labelling according Regulation (CE) No 1272/2008

Pictogram

Warning



SGH07 SGH08

Hazard statement

H302 Harmful if swallowed

H351 Suspected of causing cancer

Precautionary statements

P260 Do not breathe dust/fume/gas/mist/vapours/spray.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

Supplemental hazard statements

No additional information.

### 2.3 Other hazards

None

## 3 . COMPOSITION / INFORMATION ON INGREDIENTS

### 3.1 Substances

**Product name** : Theobromine  
**Empirical formula** : C7H8N4O2  
**CAS NUMBER** : 83-67-0  
**Synonyms** : -  
**EC Number** :

<b>Theobromine</b>		
CAS NUMBER	Concentration	Classification
83-67-0	< 100%	Carc. 2 (H351) ; Acute Tox. 4 (H302)

For the full text of the H-statements mentioned in this section, see section 16.

### 3.2 Mixtures

Not applicable

## 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.

#### Inhalation

In case of inhalation, move the victim to fresh air. If breathing is difficult, put the victim on oxygen. If breathing stops, carry out artificial respiration.

#### In case of skin contact

Wash thoroughly with water and soap.

#### In case of eye contact

Rinse well with plenty of water for at least 15 minutes.

#### Ingestion

Do not make an unconscious person vomit or swallow anything. Rinse the mouth thoroughly with water.

### 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

Carbon dioxide, dry powder.

### 5.2 Special hazards arising from the substance

Harmful/toxic vapours, carbon oxides may be released during the fire.

### 5.3 Advise for fire-fighters

Wear an autonomous breathing apparatus and suitable protection clothing against chemical agents.

## 6 . ACCIDENTAL RELEASE MEASURES

### 6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Evacuate the personnel from the contaminated zone. Ensure adequate ventilation.

### 6.2 Environmental precautions

Keeping away from drains, surface and ground waters.

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

Clean up without creating dust and place in adapted and sealed containers for elimination. Wash the contaminated area with water and soap. Confine washing water and dispose of it complying with the local regulations. After cleaning, quickly eliminate traces of water with a product absorbing liquids (for example : sand, sawdust, universal binder, Kieselguhr).

### 6.4 Reference to other sections

For disposal see section 13.

## 7 . HANDLING AND STORAGE

### 7.1 Precautions for safe handling

Avoid formation of dust. Avoid contact with skin and eyes. During handling, wear suitable personal protective equipment (see section 8). Follow the normal measures for preventive fire protection.

### 7.2 Specific handling

No data available.

### 7.3 Conditions for safe storage, including any incompatibilities

Store in a cool well-ventilated place.  
Keep container tightly closed in a dry place away from light.  
Store at <+8°C

#### 7.4 Specific end use(s)

No data available

## 8 . EXPOSURE CONTROL/PERSONAL PROTECTION

### 8.1 Control parameters

#### Occupational exposure limit values (Workplace Exposure Limits)

This information is not available.

### 8.2 Exposure controls

#### Respiratory protection

Wear imperatively an appropriated mask/respirator, tested and approved by standards such as NIOSH (US) or GEN (EU).

#### Hand protection

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

#### Eye protection

Wear safety glasses.

#### Skin protection

Wear suitable protective clothing according to the quantity and the level of activity of the substance at the workplace.

## 9 . PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

a	Physical state	: Powder
b	Odour	: No data available
c	Odour threshold	: No data available
d	pH	: No data available
e	Melting point/freezing point	: No data available
f	Initial boiling point/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	Solubility	: No data available
o	Partition coefficient: n-octanol/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 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 hazardous reactions during storage and handling complying with the instructions.

**10.4 Conditions to avoid**

No data available.

**10.5 Incompatible materials**

No data available.

**10.6 Hazardous decomposition products**

No hazardous decomposition products if the instructions for handling and storage are respected. During high overheating of the substance or during a fire, hazardous decomposition products may be produced.

**11 . TOXICOLOGICAL INFORMATION****11.1 Information on hazard classes as defined in Regulation (EC) No 1272/2008****Acute oral toxicity**

Exposure route	Result	Species	
oral	LD50, Dose : 1265 mg/kg (RTECS)	Rat	

**Acute dermal toxicity**

No data available.

**Acute inhalation toxicity**

No data available.

**Skin Corrosion**

No data available.

**Skin Irritation**

No data available.

**Serious Eye Damage**

No data available.

**Eye Irritation**

No data available.

**Respiratory Sensitisation**

No data available.

**Skin Sensitisation**

No data available.

**Germ Cell Mutagenicity**

No data available.

**Carcinogenicity**

No data available.

**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.

**11.2 Information on other hazards**

No data available.

**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 Endocrine disrupting properties

No data available.

### 12.7 Other adverse effects

No data available.

## 13 . DISPOSAL CONSIDERATIONS

### 13.1 Waste treatment methods

Non-recyclable surplus and solutions must be sent to a licensed professional waste disposal service, while respecting the local statutory instructions. Contaminated packaging is to be eliminated in the same way as the product that is contained.

## 14 . TRANSPORT INFORMATION

### 14.1 UN number or ID number

Not subject to transport regulations

### 14.2 UN proper shipping name

Not assigned.

### 14.3 Transport hazard classes

-

### 14.4 Packing group

-

### 14.5 Environmental hazards

No

### 14.6 Special precautions for user

There is no additional information.

### 14.7 Maritime transport in bulk according to IMO instruments

The cargo is not intended to be carried in bulk.

## 15 . REGULATORY INFORMATION

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

Directive 96/82/CE (SEVESO category/named substances) : not applicable.  
Regulation CE 2037/2000 (substances that deplete the ozone layer) : not applicable.  
Regulation 850/2004 (persistent organic pollutants) : not applicable.  
Regulation REACH-Titre VII (authorisations) et Titre VIII (restrictions) : not applicable.

### 15.2 Chemical safety assessment

Not applicable.

## 16 . OTHER INFORMATION

### Use

The information contained in this safety data sheet are based on our experience and our current knowledge. The data may in no case be considered as product specifications. It is provided for information purposes only with no obligation on our part. In this respect, we shall not be held liable for the use which is made of our products and for the information given above.

### Abbreviations and acronyms

ADR: Agreement on Dangerous Goods by Road  
RID: Regulations concerning the International Transport of Dangerous Goods by Rail  
IATA: International Air Transport Association  
CAS: Chemical Abstract Service  
PBT: Persistent, Bioaccumulative and Toxic  
vPvB: Very Persistent and Very Bioaccumulative

**Full text of R-phrase(s) and S-phrase(s) according to European Directive 67/548/EEC-Full text of hazard statement(s) mentioned in section 3**

**Acute Tox.** Acute oral toxicity  
**Carc.** Carcinogenictiy  
    **2** Category 2  
    **4** Category 4  
**H302** Harmful if swallowed  
**H351** Suspected of causing cancer