

# Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH)



## Theobromine ROTICHROM® CHR ≥99 %, Ph. Eur., for biochemistry

article number: **8963**  
Version: **3.0 en**  
Replaces version of: 2020-10-27  
Version: (2)

date of compilation: 2016-06-13  
Revision: 2022-01-05

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

#### 1.1 Product identifier

Identification of the substance	<b>Theobromine</b> ROTICHROM® CHR ≥99 %, Ph. Eur., for biochemistry
Article number	8963
Registration number (REACH)	It is not required to list the identified uses because the substance is not subject to registration according to REACH (< 1 t/a).
EC number	201-494-2
CAS number	83-67-0

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

Relevant identified uses:	Laboratory chemical Laboratory and analytical use
Uses advised against:	Do not use for products which come into contact with foodstuffs. Do not use for private purposes (household).

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

Carl Roth GmbH + Co KG  
Schoemperlenstr. 3-5  
D-76185 Karlsruhe  
Germany

**Telephone:**+49 (0) 721 - 56 06 0  
**Telefax:** +49 (0) 721 - 56 06 149  
**e-mail:** [sicherheit@carlroth.de](mailto:sicherheit@carlroth.de)  
**Website:** [www.carlroth.de](http://www.carlroth.de)

Competent person responsible for the safety data sheet: :Department Health, Safety and Environment

**e-mail (competent person):** [sicherheit@carlroth.de](mailto:sicherheit@carlroth.de)

#### 1.4 Emergency telephone number

Name	Street	Postal code/city	Telephone	Website
National Poisons Information Service City Hospital	Dudley Rd	B187QH Birmingham	844 892 0111	

# Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH)



Theobromine ROTICHROM® CHR ≥99 %, Ph. Eur., for biochemistry

article number: 8963

## SECTION 2: Hazards identification

### 2.1 Classification of the substance or mixture

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

Section	Hazard class	Cat-egory	Hazard class and category	Hazard statement
3.10	Acute toxicity (oral)	4	Acute Tox. 4	H302

For full text of abbreviations: see SECTION 16

### 2.2 Label elements

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

**Signal word**

**Warning**

**Pictograms**

GHS07



**Hazard statements**

H302

Harmful if swallowed

**Precautionary statements**

**Precautionary statements - prevention**

P270

Do not eat, drink or smoke when using this product

**Labelling of packages where the contents do not exceed 125 ml**

Signal word: **Warning**

Symbol(s)



### 2.3 Other hazards

**Results of PBT and vPvB assessment**

According to the results of its assessment, this substance is not a PBT or a vPvB.

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Name of substance	Theobromine
Molecular formula	C <sub>7</sub> H <sub>8</sub> N <sub>4</sub> O <sub>2</sub>
Molar mass	180,2 g/mol
CAS No	83-67-0
EC No	201-494-2

# Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH)



Theobromine ROTICHROM® CHR ≥99 %, Ph. Eur., for biochemistry

article number: 8963

Substance, Specific Conc. Limits, M-factors, ATE			
Specific Conc. Limits	M-Factors	ATE	Exposure route
-	-	1.265 mg/kg	oral

## SECTION 4: First aid measures

### 4.1 Description of first aid measures



#### General notes

Take off contaminated clothing.

#### Following inhalation

Provide fresh air. In all cases of doubt, or when symptoms persist, seek medical advice.

#### Following skin contact

Rinse skin with water/shower.

#### Following eye contact

Rinse cautiously with water for several minutes. In all cases of doubt, or when symptoms persist, seek medical advice.

#### Following ingestion

Rinse mouth with water (only if the person is conscious). Call a doctor.

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

Vomiting

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

none

## SECTION 5: Firefighting measures

### 5.1 Extinguishing media



#### Suitable extinguishing media

co-ordinate firefighting measures to the fire surroundings  
water, foam, dry extinguishing powder, ABC-powder

#### Unsuitable extinguishing media

water jet

### 5.2 Special hazards arising from the substance or mixture

Combustible.

#### Hazardous combustion products

In case of fire may be liberated: Nitrogen oxides (NO<sub>x</sub>), Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>)

# Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH)



**Theobromine ROTICHROM® CHR ≥99 %, Ph. Eur., for biochemistry**

article number: **8963**

## 5.3 Advice for firefighters

In case of fire and/or explosion do not breathe fumes. Fight fire with normal precautions from a reasonable distance. Wear self-contained breathing apparatus.

## SECTION 6: Accidental release measures

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



#### For non-emergency personnel

Avoid contact with skin, eyes and clothes. Do not breathe dust.

### 6.2 Environmental precautions

Keep away from drains, surface and ground water.

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

#### Advice on how to contain a spill

Covering of drains. Take up mechanically.

#### Advice on how to clean up a spill

Take up mechanically. Control of dust.

#### Other information relating to spills and releases

Place in appropriate containers for disposal.

### 6.4 Reference to other sections

Hazardous combustion products: see section 5. Personal protective equipment: see section 8. Incompatible materials: see section 10. Disposal considerations: see section 13.

## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

Avoid dust formation.

#### Measures to prevent fire as well as aerosol and dust generation

Removal of dust deposits.

#### Advice on general occupational hygiene

Wash hands before breaks and after work. Keep away from food, drink and animal feedingstuffs.

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

Store in a dry place. Keep container tightly closed.

#### Incompatible substances or mixtures

Observe hints for combined storage.

#### Protect against external exposure, such as

direct light irradiation, UV-radiation/sunlight, contact with air/oxygen

#### Consideration of other advice:

#### Ventilation requirements

Use local and general ventilation.

# Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH)



## Theobromine ROTICHROM® CHR ≥99 %, Ph. Eur., for biochemistry

article number: 8963

### Specific designs for storage rooms or vessels

Recommended storage temperature: 15 – 25 °C

### 7.3 Specific end use(s)

No information available.

## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### National limit values

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

Country	Name of agent	CAS No	Identifier	TWA [mg/m <sup>3</sup> ]	STEL [mg/m <sup>3</sup> ]	Ceiling-C [mg/m <sup>3</sup> ]	Notation	Source
GB	dust		WEL	10			i	EH40/2005
GB	dust		WEL	4			r	EH40/2005

#### Notation

Ceiling-C Ceiling value is a limit value above which exposure should not occur

i Inhalable fraction

r Respirable fraction

STEL Short-term exposure limit: a limit value above which exposure should not occur and which is related to a 15-minute period (unless otherwise specified)

TWA Time-weighted average (long-term exposure limit): measured or calculated in relation to a reference period of 8 hours time-weighted average (unless otherwise specified)

### 8.2 Exposure controls

#### Individual protection measures (personal protective equipment)

##### Eye/face protection



Use safety goggle with side protection.

##### Skin protection



##### • hand protection

Wear suitable gloves. Chemical protection gloves are suitable, which are tested according to EN 374. For special purposes, it is recommended to check the resistance to chemicals of the protective gloves mentioned above together with the supplier of these gloves. The times are approximate values from measurements at 22 °C and permanent contact. Increased temperatures due to heated substances, body heat etc. and a reduction of the effective layer thickness by stretching can lead to a considerable reduction of the breakthrough time. If in doubt, contact manufacturer. At an approx. 1.5 times larger / smaller layer thickness, the respective breakthrough time is doubled / halved. The data apply only to the pure substance. When transferred to substance mixtures, they may only be considered as a guide.

##### • type of material

NBR (Nitrile rubber)

# Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH)



## Theobromine ROTICHROM® CHR ≥99 %, Ph. Eur., for biochemistry

article number: 8963

- **material thickness**

>0,11 mm

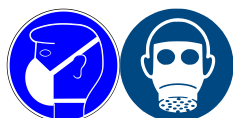
- **breakthrough times of the glove material**

>480 minutes (permeation: level 6)

- **other protection measures**

Take recovery periods for skin regeneration. Preventive skin protection (barrier creams/ointments) is recommended.

### Respiratory protection



Respiratory protection necessary at: Dust formation. Particulate filter device (EN 143). P2 (filters at least 94 % of airborne particles, colour code: White).

### Environmental exposure controls

Keep away from drains, surface and ground water.

## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

Physical state	solid
Form	powder
Colour	white
Odour	odourless
Melting point/freezing point	345 – 350 °C
Boiling point or initial boiling point and boiling range	not determined
Flammability	this material is combustible, but will not ignite readily
Lower and upper explosion limit	not determined
Flash point	not applicable
Auto-ignition temperature	>400 °C (ECHA)
Decomposition temperature	not relevant
pH (value)	not applicable
Kinematic viscosity	not relevant
<u>Solubility(ies)</u>	
Water solubility	0,5 g/l (ECHA)
<u>Partition coefficient</u>	
Partition coefficient n-octanol/water (log value):	-0,78 (ECHA)

# Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH)



## Theobromine ROTICHROM® CHR ≥99 %, Ph. Eur., for biochemistry

article number: 8963

Vapour pressure	not determined
<u>Density and/or relative density</u>	
Density	1,522 g/cm <sup>3</sup> at 20 °C
Relative vapour density	information on this property is not available
Particle characteristics	No data available.
<u>Other safety parameters</u>	
Oxidising properties	none

### 9.2 Other information

Information with regard to physical hazard classes:	hazard classes acc. to GHS (physical hazards): not relevant
Other safety characteristics:	There is no additional information.

## SECTION 10: Stability and reactivity

### 10.1 Reactivity

The product in the delivered form is not dust explosion capable; the enrichment of fine dust however leads to the danger of dust explosion.

### 10.2 Chemical stability

The material is stable under normal ambient and anticipated storage and handling conditions of temperature and pressure.

### 10.3 Possibility of hazardous reactions

**Violent reaction with:** strong oxidiser

### 10.4 Conditions to avoid

Direct light irradiation. UV-radiation/sunlight. Contact with air/oxygen.

### 10.5 Incompatible materials

There is no additional information.

### 10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.

## SECTION 11: Toxicological information

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

Classification according to GHS (1272/2008/EC, CLP)

#### Acute toxicity

Harmful if swallowed.

Acute toxicity					
Exposure route	Endpoint	Value	Species	Method	Source
oral	LD50	1.265 mg/kg	rat		TOXNET

# Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH)



## Theobromine ROTICHROM® CHR ≥99 %, Ph. Eur., for biochemistry

article number: 8963

---

### **Skin corrosion/irritation**

Shall not be classified as corrosive/irritant to skin.

### **Serious eye damage/eye irritation**

Shall not be classified as seriously damaging to the eye or eye irritant.

### **Respiratory or skin sensitisation**

Shall not be classified as a respiratory or skin sensitiser.

### **Germ cell mutagenicity**

Shall not be classified as germ cell mutagenic.

### **Carcinogenicity**

Shall not be classified as carcinogenic.

### **Reproductive toxicity**

Shall not be classified as a reproductive toxicant.

### **Specific target organ toxicity - single exposure**

Shall not be classified as a specific target organ toxicant (single exposure).

### **Specific target organ toxicity - repeated exposure**

Shall not be classified as a specific target organ toxicant (repeated exposure).

### **Aspiration hazard**

Shall not be classified as presenting an aspiration hazard.

## **Symptoms related to the physical, chemical and toxicological characteristics**

### **• If swallowed**

diarrhoea, vomiting, nausea, dizziness

### **• If in eyes**

Data are not available.

### **• If inhaled**

Data are not available.

### **• If on skin**

Data are not available.

### **• Other information**

none

## **11.2 Endocrine disrupting properties**

Not listed.

## **11.3 Information on other hazards**

There is no additional information.



# Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH)



Theobromine ROTICHROM® CHR ≥99 %, Ph. Eur., for biochemistry

article number: 8963

## SECTION 12: Ecological information

### 12.1 Toxicity

Shall not be classified as hazardous to the aquatic environment.

Aquatic toxicity (acute)				
Endpoint	Value	Species	Source	Exposure time
EC50	>100 mg/l	aquatic invertebrates	ECHA	48 h
ErC50	>100 mg/l	algae	ECHA	72 h

### Biodegradation

The substance is readily biodegradable.

### 12.2 Process of degradability

Theoretical Oxygen Demand with nitrification: 1,476 mg/mg

Theoretical Oxygen Demand: 0,888 mg/mg

Theoretical Carbon Dioxide: 1,71 mg/mg

### 12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW)	-0,78 (ECHA)
---------------------------	--------------

### 12.4 Mobility in soil

Data are not available.

### 12.5 Results of PBT and vPvB assessment

Data are not available.

### 12.6 Endocrine disrupting properties

Not listed.

### 12.7 Other adverse effects

Data are not available.

## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods



This material and its container must be disposed of as hazardous waste. Dispose of contents/container in accordance with local/regional/national/international regulations.

#### Sewage disposal-relevant information

Do not empty into drains.

### 13.2 Relevant provisions relating to waste

The allocation of waste identity numbers/waste descriptions must be carried out according to the EEC, specific to the industry and process. Waste catalogue ordinance (Germany).

# Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH)



## Theobromine ROTICHROM® CHR ≥99 %, Ph. Eur., for biochemistry

article number: 8963

### 13.3 Remarks

Waste shall be separated into the categories that can be handled separately by the local or national waste management facilities. Please consider the relevant national or regional provisions.

## SECTION 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 class(es)** none
- 14.4 Packing group** not assigned
- 14.5 Environmental hazards** non-environmentally hazardous acc. to the dangerous goods regulations
- 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.

### 14.8 Information for each of the UN Model Regulations

#### Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN) - Additional information

Not subject to ADR, RID and ADN.

#### International Maritime Dangerous Goods Code (IMDG) - Additional information

Not subject to IMDG.

#### International Civil Aviation Organization (ICAO-IATA/DGR) - Additional information

Not subject to ICAO-IATA.

## SECTION 15: Regulatory information

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

#### Relevant provisions of the European Union (EU)

#### Restrictions according to REACH, Annex XVII

not listed

#### List of substances subject to authorisation (REACH, Annex XIV)/SVHC - candidate list

Not listed.

#### Seveso Directive

2012/18/EU (Seveso III)			
No	Dangerous substance/hazard categories	Qualifying quantity (tonnes) for the application of lower and upper-tier requirements	Notes
	not assigned		

#### Deco-Paint Directive

# Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH)



## Theobromine ROTICHROM® CHR ≥99 %, Ph. Eur., for biochemistry

article number: 8963

VOC content	0 % , 0 g/l
-------------	----------------

### Industrial Emissions Directive (IED)

VOC content	0 %
VOC content	0 g/l

### Directive on the restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS)

not listed

### Regulation concerning the establishment of a European Pollutant Release and Transfer Register (PRTR)

not listed

### Water Framework Directive (WFD)

List of pollutants (WFD)				
Name of substance	Name acc. to inventory	CAS No	Listed in	Remarks
Theobromine	Substances and preparations, or the breakdown products of such, which have been proved to possess carcinogenic or mutagenic properties or properties which may affect steroidogenic, thyroid, reproduction or other endocrine-related functions in or via the aquatic environment		A)	

#### Legend

A) Indicative list of the main pollutants

### Regulation on the marketing and use of explosives precursors

not listed

### Regulation on drug precursors

not listed

### Regulation on substances that deplete the ozone layer (ODS)

not listed

### Regulation concerning the export and import of hazardous chemicals (PIC)

not listed

### Regulation on persistent organic pollutants (POP)

not listed

### Other information

Directive 94/33/EC on the protection of young people at work. Observe employment restrictions under the Maternity Protection Directive (92/85/EEC) for expectant or nursing mothers.

# Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH)



## Theobromine ROTICHROM® CHR ≥99 %, Ph. Eur., for biochemistry

article number: 8963

### National inventories

Country	Inventory	Status
AU	AICS	substance is listed
CA	NDSL	substance is listed
CN	IECSC	substance is listed
EU	ECSI	substance is listed
EU	REACH Reg.	substance is listed
JP	CSCL-ENCS	substance is listed
JP	ISHA-ENCS	substance is listed
KR	KECI	substance is listed
NZ	NZIoC	substance is listed
PH	PICCS	substance is listed
TW	TCSI	substance is listed
US	TSCA	substance is listed

#### Legend

AICS	Australian Inventory of Chemical Substances
CSCL-ENCS	List of Existing and New Chemical Substances (CSCL-ENCS)
ECSI	EC Substance Inventory (EINECS, ELINCS, NLP)
IECSC	Inventory of Existing Chemical Substances Produced or Imported in China
ISHA-ENCS	Inventory of Existing and New Chemical Substances (ISHA-ENCS)
KECI	Korea Existing Chemicals Inventory
NDSL	Non-domestic Substances List (NDSL)
NZIoC	New Zealand Inventory of Chemicals
PICCS	Philippine Inventory of Chemicals and Chemical Substances (PICCS)
REACH Reg.	REACH registered substances
TCSI	Taiwan Chemical Substance Inventory
TSCA	Toxic Substance Control Act

### 15.2 Chemical Safety Assessment

No Chemical Safety Assessment has been carried out for this substance.

## SECTION 16: Other information

### Indication of changes (revised safety data sheet)

Alignment to regulation: Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU

Restructuring: section 9, section 14

Section	Former entry (text/value)	Actual entry (text/value)	Safety-relevant
2.1		Classification according to Regulation (EC) No 1272/2008 (CLP): change in the listing (table)	yes
2.3	Other hazards: There is no additional information.	Other hazards	yes
2.3		Results of PBT and vPvB assessment: According to the results of its assessment, this substance is not a PBT or a vPvB.	yes

# Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH)



## Theobromine ROTICHROM® CHR ≥99 %, Ph. Eur., for biochemistry

article number: 8963

### Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
ADN	Accord européen relatif au transport international des marchandises dangereuses par voies de navigation intérieures (European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways)
ADR	Accord relatif au transport international des marchandises dangereuses par route (Agreement concerning the International Carriage of Dangerous Goods by Road)
ATE	Acute Toxicity Estimate
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
Ceiling-C	Ceiling value
CLP	Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures
DGR	Dangerous Goods Regulations (see IATA/DGR)
EC50	Effective Concentration 50 %. The EC50 corresponds to the concentration of a tested substance causing 50 % changes in response (e.g. on growth) during a specified time interval
EC No	The EC Inventory (EINECS, ELINCS and the NLP-list) is the source for the seven-digit EC number, an identifier of substances commercially available within the EU (European Union)
EH40/2005	EH40/2005 Workplace exposure limits ( <a href="http://www.nationalarchives.gov.uk/doc/open-government-licence/">http://www.nationalarchives.gov.uk/doc/open-government-licence/</a> )
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
ErC50	≡ EC50: in this method, that concentration of test substance which results in a 50 % reduction in either growth (EbC50) or growth rate (ErC50) relative to the control
GHS	"Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Nations
IATA	International Air Transport Association
IATA/DGR	Dangerous Goods Regulations (DGR) for the air transport (IATA)
ICAO	International Civil Aviation Organization
IMDG	International Maritime Dangerous Goods Code
LD50	Lethal Dose 50 %: the LD50 corresponds to the dose of a tested substance causing 50 % lethality during a specified time interval
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RID	Règlement concernant le transport International ferroviaire des marchandises Dangereuses (Regulations concerning the International carriage of Dangerous goods by Rail)
STEL	Short-term exposure limit
SVHC	Substance of Very High Concern
TWA	Time-weighted average
VOC	Volatile Organic Compounds
vPvB	Very Persistent and very Bioaccumulative
WEL	Workplace exposure limit

# Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH)



## Theobromine ROTICHROM® CHR ≥99 %, Ph. Eur., for biochemistry

article number: **8963**

### Key literature references and sources for data

Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures.  
Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU.

Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN). International Maritime Dangerous Goods Code (IMDG). Dangerous Goods Regulations (DGR) for the air transport (IATA).

### List of relevant phrases (code and full text as stated in section 2 and 3)

Code	Text
H302	Harmful if swallowed.

### Disclaimer

This information is based upon the present state of our knowledge. This SDS has been compiled and is solely intended for this product.