

# Safety data sheet

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



## Caffeine ROTI®CALIPURE anhydrous, Melting point standard, 235-238 °C

article number: **9739**  
Version: **5.0 en**  
Replaces version of: 05.01.2022  
Version: (4)

date of compilation: 27.08.2015  
Revision: 04.03.2024

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

### 1.1 Product identifier

Identification of the substance	<b>Caffeine ROTI®CALIPURE</b> anhydrous, Melting point standard, 235-238 °C
Article number	9739
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).
Index number in CLP Annex VI	613-086-00-5
EC number	200-362-1
CAS number	58-08-2

### 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 private purposes (household). Food, drink and animal feedingstuffs.

### 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  
**Website:** 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

## 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

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## 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.

### Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of  $\geq 0,1\%$ .

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Name of substance	Caffeine
Molecular formula	$C_8H_{10}N_4O_2$
Molar mass	194,2 g/mol
CAS No	58-08-2
EC No	200-362-1
Index No	613-086-00-5

Substance, Specific Conc. Limits, M-factors, ATE			
Specific Conc. Limits	M-Factors	ATE	Exposure route
-	-	367,7 mg/kg	oral

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## 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.

#### 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

Agitation, Headache, Diarrhoea, Vomiting, Blood pressure drop, Circulatory collapse

### 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, alcohol resistant 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>)

### 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.

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## 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. Retain contaminated washing water and dispose of it.

### 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.

#### Incompatible substances or mixtures

Observe hints for combined storage.

#### Consideration of other advice:

#### Ventilation requirements

Use local and general ventilation.

#### Specific designs for storage rooms or vessels

Recommended storage temperature: 15 – 25 °C

### 7.3 Specific end use(s)

No information available.

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## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### National limit values

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

This information is not available.

#### Human health values

Relevant DNELs and other threshold levels				
Endpoint	Threshold level	Protection goal, route of exposure	Used in	Exposure time
DNEL	44,37 mg/m <sup>3</sup>	human, inhalatory	worker (industry)	chronic - systemic effects
DNEL	25,17 mg/kg bw/day	human, dermal	worker (industry)	chronic - systemic effects

#### Environmental values

Relevant PNECs and other threshold levels				
End-point	Threshold level	Organism	Environmental compartment	Exposure time
PNEC	0,087 mg/l	aquatic organisms	freshwater	short-term (single instance)
PNEC	0,009 mg/l	aquatic organisms	marine water	short-term (single instance)
PNEC	10 mg/l	aquatic organisms	sewage treatment plant (STP)	short-term (single instance)
PNEC	0,4 mg/kg	aquatic organisms	freshwater sediment	short-term (single instance)
PNEC	0,029 mg/kg	terrestrial organisms	soil	short-term (single instance)

### 8.2 Exposure controls

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

##### Eye/face protection



Use safety goggle with side protection.

##### Skin protection



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### • 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)

### • 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, crystalline
Colour	white
Odour	odourless
Melting point/freezing point	236 – 239 °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	not determined
Decomposition temperature	not relevant

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pH (value)	5,5 – 6,5 (in aqueous solution: 10 g/l, 20 °C)
Kinematic viscosity	not relevant
<u>Solubility(ies)</u>	
Water solubility	20 g/l at 20 °C
<u>Partition coefficient</u>	
Partition coefficient n-octanol/water (log value):	-0,091 (23 °C) (ECHA)
Soil organic carbon/water (log KOC)	1 (ECHA)
Vapour pressure	not determined
<u>Density and/or relative density</u>	
Density	1,23 g/cm <sup>3</sup> at 18 °C
Relative vapour density	Information on this property is not available.
Bulk density	200 – 250 kg/m <sup>3</sup>
Particle characteristics	No data available.
<u>Other safety parameters</u>	
Oxidising properties	none
<b>9.2 Other information</b>	
Information with regard to physical hazard classes:	hazard classes acc. to GHS (physical hazards): not relevant
Other safety characteristics:	
Temperature class (EU, acc. to ATEX)	T1 Maximum permissible surface temperature on the equipment: 450°C

## 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

Keep away from heat.

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## 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	367,7 mg/kg	rat		ECHA
dermal	LD50	>2.000 mg/kg	rat		ECHA

#### 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

- **If in eyes**

essentially non-irritating



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- **If inhaled**

Data are not available.

- **If on skin**

essentially non-irritating

- **Other information**

Other adverse effects: Agitation, Headache, Blood pressure drop, Circulatory collapse

### 11.2 Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of  $\geq 0,1\%$ .

### 11.3 Information on other hazards

There is no additional information.

## 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
LC50	87 mg/l	fish	ECHA	96 h
EC50	182 mg/l	aquatic invertebrates	ECHA	48 h
ErC50	>100 mg/l	algae	ECHA	72 h

Aquatic toxicity (chronic)				
Endpoint	Value	Species	Source	Exposure time
EC50	3.490 mg/l	microorganisms	ECHA	17 h

### 12.2 Persistence and degradability

Theoretical Oxygen Demand (without nitrification): 1,071 mg/mg

Theoretical Oxygen Demand (with nitrification): 1,617 mg/mg

Theoretical Carbon Dioxide: 1,813 mg/mg

#### Biodegradation

The substance is readily biodegradable.

Process of degradability		
Process	Degradation rate	Time
biotic/abiotic	90 - 100 %	22 d
DOC removal	>90 - 100 %	22 d

### 12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW)	-0,091 (23 °C) (ECHA)
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### 12.4 Mobility in soil

Henry's law constant	0 Pa m <sup>3</sup> /mol at 25 °C (ECHA)
The Organic Carbon normalised adsorption coefficient	1 (ECHA)

### 12.5 Results of PBT and vPvB assessment

Data are not available.

### 12.6 Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of  $\geq 0,1\%$ .

### 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.

#### Waste treatment of containers/packagings

Handle contaminated packages in the same way as the substance itself. Completely emptied packages can be recycled.

### 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.

#### Properties of waste which render it hazardous

**HP 6** acute toxicity

### 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. Non-contaminated packages may be recycled.

## 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	

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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

### 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

VOC content	0 %
VOC content	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

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### Water Framework Directive (WFD)

List of pollutants (WFD)				
Name of substance	Name acc. to inventory	CAS No	Listed in	Remarks
Caffeine	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.

### National inventories

Country	Inventory	Status
AU	AIIC	substance is listed
CA	DSL	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
KR	KECI	substance is listed
MX	INSQ	substance is listed
NZ	NZIoC	substance is listed
PH	PICCS	substance is listed
TR	CICR	substance is listed
TW	TCSI	substance is listed

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Country	Inventory	Status
US	TSCA	substance is listed (ACTIVE)
VN	NCI	substance is listed

### Legend

AIIC	Australian Inventory of Industrial Chemicals
CICR	Chemical Inventory and Control Regulation
CSCL-ENCS	List of Existing and New Chemical Substances (CSCL-ENCS)
DSL	Domestic Substances List (DSL)
ECSI	EC Substance Inventory (EINECS, ELINCS, NLP)
IECSC	Inventory of Existing Chemical Substances Produced or Imported in China
INSQ	National Inventory of Chemical Substances
KECI	Korea Existing Chemicals Inventory
NCI	National Chemical Inventory
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)

Section	Former entry (text/value)	Actual entry (text/value)	Safety-relevant
2.3		Endocrine disrupting properties: Does not contain an endocrine disruptor (ED) at a concentration of $\geq 0,1\%$ .	yes
14.8	Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN) - Additional information: Not subject to ADR, RID and ADN.		yes
15.1	VOC content: 0 % , 0 g/l	VOC content: 0 %	yes
15.1		VOC content: 0 g/l	yes
15.1		National inventories: change in the listing (table)	yes

### Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
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)
CLP	Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures
DGR	Dangerous Goods Regulations (see IATA/DGR)
DNEL	Derived No-Effect Level

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Abbr.	Descriptions of used abbreviations
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)
ED	Endocrine disruptor
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
index No	The Index number is the identification code given to the substance in Part 3 of Annex VI to Regulation (EC) No 1272/2008
LC50	Lethal Concentration 50%: the LC50 corresponds to the concentration of a tested substance causing 50 % lethality during a specified time interval
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
PNEC	Predicted No-Effect Concentration
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SVHC	Substance of Very High Concern
VOC	Volatile Organic Compounds
vPvB	Very Persistent and very Bioaccumulative

### 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.

Agreement concerning the International Carriage of Dangerous Goods by Road (ADR). 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.