

Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU



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

article number: **9739**
Version: **3.0 en**
Replaces version of: 25.01.2019
Version: (2)

date of compilation: 27.08.2015
Revision: 27.10.2020

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

1.1 Product identifier

Identification of the substance	Caffeine ROTI®CALIPURE 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 No	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

Identified uses:	laboratory chemical laboratory and analytical use
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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

1.4 Emergency telephone number

Emergency information service **Poison Centre Munich: +49/(0)89 19240**

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

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

Classification acc. to GHS			
Section	Hazard class	Hazard class and category	Hazard statement
3.10	acute toxicity (oral)	(Acute Tox. 4)	H302

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

There is no additional information.

SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance	Caffeine
Index No	613-086-00-5
EC number	200-362-1
CAS number	58-08-2
Molecular formula	C ₈ H ₁₀ N ₄ O ₂
Molar mass	194,2 g/mol

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.

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Following skin contact

Rinse skin with water/shower.

Following eye contact

Rinse cautiously with water for several minutes.

Following ingestion

Rinse mouth immediately and drink plenty of water. 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 fire-fighting measures to the fire surroundings
water spray, foam, dry extinguishing powder, carbon dioxide (CO₂)

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_x), carbon monoxide (CO), carbon dioxide (CO₂)

5.3 Advice for firefighters

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

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

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.

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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

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

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed. 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.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

National limit values

Occupational exposure limit values (Workplace Exposure Limits)

Data are not available.

Relevant DNELs/DMELs/PNECs and other threshold levels

• human health values

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

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• environmental values

Endpoint	Threshold level	Environmental compartment	Exposure time
PNEC	0,087 mg/l	freshwater	short-term (single instance)
PNEC	0,009 mg/l	marine water	short-term (single instance)
PNEC	10 mg/l	sewage treatment plant (STP)	short-term (single instance)
PNEC	0,4 mg/kg	freshwater sediment	short-term (single instance)
PNEC	0,029 mg/kg	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



• 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).

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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

Appearance

Physical state	solid (powder, crystalline)
Colour	white
Odour	odourless
Odour threshold	no data available

Other physical and chemical parameters

pH (value)	5,5 – 6,5 (water: 10 g/l, 20 °C)
Melting point/freezing point	236 – 239 °C
Initial boiling point and boiling range	this information is not available
Flash point	not applicable
Evaporation rate	no data available
Flammability (solid, gas)	these information are not available
<u>Explosive limits</u>	
• lower explosion limit (LEL)	this information is not available
• upper explosion limit (UEL)	this information is not available
Explosion limits of dust clouds	these information are not available
Vapour pressure	this information is not available
Density	1,23 g/cm ³ at 18 °C
Vapour density	this information is not available
Bulk density	200 – 250 kg/m ³
Relative density	this information is not available
<u>Solubility(ies)</u>	
Water solubility	~ 20 g/l at 20 °C
<u>Partition coefficient</u>	
n-octanol/water (log KOW)	-0,091 (23 °C) (ECHA)
Soil organic carbon/water (log KOC)	1 (ECHA)
Auto-ignition temperature	>500 °C
Decomposition temperature	no data available
Viscosity	not relevant (solid matter)
Explosive properties	Shall not be classified as explosive.
Oxidising properties	none

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9.2 Other information

Temperature class (EU, acc. to ATEX)

T1 (Maximum permissible surface temperature on the equipment: 450°C)

SECTION 10: Stability and reactivity

10.1 Reactivity

Dust explosibility.

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.

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 toxicological effects

Acute toxicity

Exposure route	Endpoint	Value	Species	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.

Summary of evaluation of the CMR properties

Shall not be classified as germ cell mutagenic, carcinogenic nor 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.

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Symptoms related to the physical, chemical and toxicological characteristics

• **If swallowed**

vomiting, diarrhoea

• **If in eyes**

essentially non-irritating

• **If inhaled**

data are not available

• **If on skin**

essentially non-irritating

Other information

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

SECTION 12: Ecological information

12.1 Toxicity

acc. to 1272/2008/EC: 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
growth (EbCx) 10%	1.530 mg/l	microorganisms	ECHA	17 h

12.2 Process of degradability

The substance is readily biodegradable.

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

Theoretical Oxygen Demand: 1,071 mg/mg

Theoretical Carbon Dioxide: 1,813 mg/mg

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)

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12.4 Mobility in soil

Henry's law constant	$0 \text{ Pa m}^3/\text{mol}$ at 25 °C
The Organic Carbon normalised adsorption coefficient	1

12.5 Results of PBT and vPvB assessment

Data are not available.

12.6 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.

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	(not subject to transport regulations)
14.2	UN proper shipping name	not relevant
14.3	Transport hazard class(es)	not relevant
	Class	-
14.4	Packing group	not relevant, not assigned to a packing group
14.5	Environmental hazards	NONE (non-environmentally hazardous acc. to the dangerous goods regulations)
14.6	Special precautions for user	There is no additional information.
14.7	Transport in bulk according to Annex II of MARPOL and the IBC Code	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)	Not subject to ADR, RID and ADN.

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- **International Maritime Dangerous Goods Code (IMDG)**

Not subject to IMDG.

- **International Civil Aviation Organization (ICAO-IATA/DGR)**

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)

- **Regulation 649/2012/EU concerning the export and import of hazardous chemicals (PIC)**

Not listed.

- **Regulation 1005/2009/EC on substances that deplete the ozone layer (ODS)**

Not listed.

- **Regulation 850/2004/EC on persistent organic pollutants (POP)**

Not listed.

- **Restrictions according to REACH, Annex XVII**

not listed

Name acc. to inventory	CAS No	Wt%	Listed in	Remarks
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		100	A)	

Legend

A) Indicative list of the main pollutants

- **Restrictions according to REACH, Title VIII**

None.

- **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		

- **Directive 75/324/EEC relating to aerosol dispensers**

Filling batch

Deco-Paint Directive (2004/42/EC)

VOC content	0 % 0 g/l
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Directive on industrial emissions (VOCs, 2010/75/EU)

VOC content	0 %
VOC content	0 g/l

Directive 2011/65/EU on the restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS) - Annex II

not listed

Regulation 166/2006/EC concerning the establishment of a European Pollutant Release and Transfer Register (PRTR)

not listed

Directive 2000/60/EC establishing a framework for Community action in the field of water policy (WFD)

Name acc. to inventory	CAS No	Listed in	Remarks
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 98/2013/EU on the marketing and use of explosives precursors

not listed

Regulation 111/2005/EC laying down rules for the monitoring of trade between the Community and third countries in drug precursors

not listed

National inventories

Substance is listed in the following national inventories:

Country	National inventories	Status
AU	AICS	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
US	TSCA	substance is listed

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Legend

AICS	Australian Inventory of Chemical Substances
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
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
8.1		• environmental values: change in the listing (table)	yes
14.4	Packing group: not relevant	Packing group: not relevant, not assigned to a packing group	yes

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 européen relatif au transport international des marchandises dangereuses par route (European Agreement concerning the International Carriage of Dangerous Goods by Road)
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
CMR	Carcinogenic, Mutagenic or toxic for Reproduction
DGR	Dangerous Goods Regulations (see IATA/DGR)
DMEL	Derived Minimal Effect Level
DNEL	Derived No-Effect Level
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
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

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Abbr.	Descriptions of used abbreviations
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
MARPOL	International Convention for the Prevention of Pollution from Ships (abbr. of "Marine Pollutant")
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No-Effect Concentration
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)
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. 1907/2006 (REACH), amended by 2015/830/EU
- Regulation (EC) No. 1272/2008 (CLP, EU GHS)
- Dangerous Goods Regulations (DGR) for the air transport (IATA)
- International Maritime Dangerous Goods Code (IMDG)

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

Code	Text
H302	harmful if swallowed

Disclaimer

The above information describes exclusively the safety requirements of the product and is based on our present-day knowledge. The information is intended to give you advice about the safe handling of the product named in this safety data sheet, for storage, processing, transport and disposal. The information cannot be transferred to other products. In the case of mixing the product with other products or in the case of processing, the information on this safety data sheet is not necessarily valid for the new made-up material.