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Article: 2921 Melting point standard Set 1 ROTI®Calipure

Date of compilation: 2022-05-16

1 Composition/information on ingredients

Bill of materials

| Name of substance | Identifier | Number of pieces | Classification acc. to GHS | Pictograms | Page |
|-------------------|--|------------------|----------------------------|---|---------|
| Vanillin | CAS No 121-33-5 EC No 204-465-2 Article number 9714 | 1 | Eye Irrit. 2 / H319 |  | 4 – 17 |
| Sulphanilamide | CAS No 63-74-1 EC No 200-563-4 Article number 9734 | 1 | | | 18 – 29 |
| Caffeine | CAS No 58-08-2 EC No 200-362-1 Article number 9739 | 1 | Acute Tox. 4 / H302 |  | 30 – 44 |

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2 Hazards identification

2.1 Label elements

Signal word Warning

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

Pictograms

Warning.



Hazard statement(s)

| | |
|------|-------------------------------|
| H302 | Harmful if swallowed |
| H319 | Causes serious eye irritation |

Precautionary statements

Precautionary statements - prevention

| | |
|------|---------------------------------------|
| P280 | Wear protective gloves/eye protection |
|------|---------------------------------------|

Precautionary statements - response

| | |
|----------------|---|
| P301+P312 | IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell |
| P305+P351+P338 | IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing |
| P337+P313 | If eye irritation persists: Get medical advice/attention |

3 Transport information

- | | |
|--|---|
| 3.1 UN number or ID number | not subject to transport regulations |
| 3.2 UN proper shipping name | not assigned |
| 3.3 Transport hazard class(es) | none |
| 3.4 Packing group | not assigned |
| 3.5 Environmental hazards | non-environmentally hazardous acc. to the dangerous goods regulations |
| 3.6 Special precautions for user | There is no additional information. |
| 3.7 Maritime transport in bulk according to IMO instruments | The cargo is not intended to be carried in bulk. |
| 3.8 Information for each of the UN Model Regulations | |
| Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN) - Additional information | not assigned |
| International Maritime Dangerous Goods Code (IMDG) - Additional information | Not subject to IMDG. |



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International Civil Aviation Organization (ICAO-IATA/DGR) - Additional information
Not subject to ICAO-IATA.

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



Vanillin ROTI®CALIPURE 81-83 °C Melting point standard

article number: **9714**
Version: **3.0 en**
Replaces version of: 2019-04-29
Version: (2)

date of compilation: 2015-08-28
Revision: 2022-05-16

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

1.1 Product identifier

| | |
|---------------------------------|---|
| Identification of the substance | Vanillin ROTI®CALIPURE 81-83 °C Melting point standard |
| Article number | 9714 |
| EC number | 204-465-2 |
| CAS number | 121-33-5 |
| Alternative name(s) | 4-Hydroxy-3-methoxybenzaldehyde |

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
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

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

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification acc. to GHS

| Section | Hazard class | Cat-egory | Hazard class and category | Hazard statement |
|---------|-----------------------------------|-----------|---------------------------|------------------|
| 3.3 | Serious eye damage/eye irritation | 2 | Eye Irrit. 2 | H319 |

For full text of abbreviations: see SECTION 16

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2.2 Label elements

Labelling

Signal word

Warning

Pictograms

GHS07



Hazard statements

H319 Causes serious eye irritation

Precautionary statements

Precautionary statements - prevention

P280 Wear protective gloves/eye protection

Precautionary statements - response

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
P337+P313 If eye irritation persists: Get medical advice/attention

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 | Vanillin |
| Molecular formula | C ₈ H ₈ O ₃ |
| Molar mass | 152,2 g/mol |
| CAS No | 121-33-5 |
| EC No | 204-465-2 |

SECTION 4: First aid measures

4.1 Description of first aid measures



General notes

Take off contaminated clothing.

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

Following eye contact

Irrigate copiously with clean, fresh water for at least 10 minutes, holding the eyelids apart. In case of eye irritation consult an ophthalmologist.

Following ingestion

Rinse mouth. Call a doctor if you feel unwell.

4.2 Most important symptoms and effects, both acute and delayed

Irritation

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: Carbon monoxide (CO), Carbon dioxide (CO₂)

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.

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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. Ventilate affected area.

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

Provision of sufficient ventilation. 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.

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 ³] | STEL [mg/m ³] | Ceiling-C [mg/m ³] | 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

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Notation

| | |
|------|--|
| 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) |

Environmental values

| Relevant PNECs and other threshold levels | | | | |
|---|-----------------|-----------------------|------------------------------|------------------------------|
| End-point | Threshold level | Organism | Environmental compartment | Exposure time |
| PNEC | 0,118 mg/l | aquatic organisms | freshwater | short-term (single instance) |
| PNEC | 0,012 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 | 58,22 mg/kg | aquatic organisms | freshwater sediment | short-term (single instance) |
| PNEC | 5,822 mg/kg | aquatic organisms | marine sediment | short-term (single instance) |
| PNEC | 11,54 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



• 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

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• 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). P1 (filters at least 80 % 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 | light yellow |
| Odour | characteristic |
| Melting point/freezing point | 81 – 83 °C |
| Boiling point or initial boiling point and boiling range | 285 °C at 1.013 hPa |
| Flammability | this material is combustible, but will not ignite readily |
| Lower and upper explosion limit | not determined |
| Flash point | 159,8 – 160,8 °C at 1.022 hPa (c.c.) (ECHA) |
| Auto-ignition temperature | not determined |
| Decomposition temperature | >160 °C |
| pH (value) | 4,3 (in aqueous solution: 10 g/l, 20 °C) |
| Kinematic viscosity | not relevant |
| <u>Solubility(ies)</u> | |
| Water solubility | 10 g/l at 25 °C |
| Solubility in diethyl ether | soluble |
| Solubility in ethyl acetate | soluble |
| <u>Partition coefficient</u> | |
| Partition coefficient n-octanol/water (log value): | 1,17 – 1,21 (25 °C) (exp.) |
| Soil organic carbon/water (log KOC) | 1,644 (ECHA) |

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| | |
|--|---|
| Vapour pressure | 0,0029 hPa at 25 °C |
| <u>Density and/or relative density</u> | |
| Density | 1,06 g/cm ³ at 20 °C (ECHA) |
| Relative vapour density | information on this property is not available |
| Bulk density | ~ 600 kg/m ³ |
| 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, Reducing agents, Bases

10.4 Conditions to avoid

Keep away from heat. Decomposition takes place from temperatures above: >160 °C.

10.5 Incompatible materials

aluminium

10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Classification acc. to GHS

Acute toxicity

Shall not be classified as acutely toxic.

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| Acute toxicity | | | | | |
|----------------|----------|--------------|---------|--------|--------|
| Exposure route | Endpoint | Value | Species | Method | Source |
| oral | LD50 | 3.300 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

Causes serious eye irritation.

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

Data are not available.

• If in eyes

Causes serious eye irritation

• 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.

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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 | 57 mg/l | Pimephales promelas | ECHA | 96 h |
| EC50 | 36,79 mg/l | daphnia magna | ECHA | 48 h |
| ErC50 | 120 mg/l | algae | ECHA | 72 h |

| Aquatic toxicity (chronic) | | | | |
|----------------------------|---------|-----------------------|--------|---------------|
| Endpoint | Value | Species | Source | Exposure time |
| EC50 | 16 mg/l | aquatic invertebrates | ECHA | 21 d |

Biodegradation

The substance is readily biodegradable.

12.2 Process of degradability

Theoretical Oxygen Demand: 1,788 mg/mg
Theoretical Carbon Dioxide: 2,314 mg/mg

| Process of degradability | | |
|--------------------------|------------------|------|
| Process | Degradation rate | Time |
| biotic/abiotic | 72 % | 28 d |

12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

| | |
|---------------------------|----------------------------|
| n-octanol/water (log KOW) | 1,17 - 1,21 (25 °C) (Exp.) |
|---------------------------|----------------------------|

12.4 Mobility in soil

| | |
|--|--------------|
| The Organic Carbon normalised adsorption coefficient | 1,644 (ECHA) |
|--|--------------|

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.

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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).

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 | <u>Information for each of the UN Model Regulations</u> | |
| | 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. |

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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)

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 % |
|-------------|-----|

Industrial Emissions Directive (IED)

| | |
|-------------|-----|
| VOC content | 0 % |
|-------------|-----|

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)

not listed

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

National regulations(GB)

List of substances subject to authorisation (GB REACH, Annex 14) / SVHC - candidate list

not listed

Restrictions according to GB REACH, Annex 17

not listed

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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 |
| US | TSCA | 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 |
| 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:

Restructuring: section 9, section 14

| Section | Former entry (text/value) | Actual entry (text/value) | Safety-relevant |
|---------|--|--|-----------------|
| 2.1 | | Classification acc. to GHS: change in the listing (table) | yes |
| 2.2 | Labelling of packages where the contents do not exceed 125 ml: Signal word: Warning | | yes |

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| Section | Former entry (text/value) | Actual entry (text/value) | Safety-relevant |
|---------|---|---|-----------------|
| 2.2 | | Labelling of packages where the contents do not exceed 125 ml: change in the listing (table) | yes |
| 2.2 | | Labelling of packages where the contents do not exceed 125 ml: 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 |

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) |
| CAS | Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances) |
| Ceiling-C | Ceiling value |
| 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 (http://www.nationalarchives.gov.uk/doc/open-government-licence/) |
| 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 |
| GB REACH | The REACH etc. (Amendment etc.) (EU Exit) Regulations 2019, SI 2019/758 (as amended) |
| 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 |
| 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 |

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| Abbr. | Descriptions of used abbreviations |
|-------|---|
| 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) |
| STEL | Short-term exposure limit |
| TWA | Time-weighted average |
| VOC | Volatile Organic Compounds |
| vPvB | Very Persistent and very Bioaccumulative |
| WEL | Workplace exposure limit |

Key literature references and sources for data

Agreement concerning the International Carriage of Dangerous Goods by Road (ADR). Regulations concerning the International Carriage of Dangerous Goods by Rail (RID). 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 |
|------|--------------------------------|
| H319 | Causes serious eye irritation. |

Disclaimer

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

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Sulphanilamide ROTI®CALIPURE 164-166 °C Melting point standard

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date of compilation: 2019-04-29
Revision: 2022-05-16

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

1.1 Product identifier

Identification of the substance **Sulphanilamide ROTI®CALIPURE 164-166 °C Melting point standard**

Article number 9734

EC number 200-563-4

CAS number 63-74-1

Alternative name(s) 4-Aminobenzenesulphonamide

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
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

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

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification acc. to GHS

This substance does not meet the criteria for classification.

2.2 Label elements

Labelling

not required

Safety data sheet

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



Sulphanilamide ROTI®CALIPURE 164-166 °C Melting point standard

article number: 9734

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 | Sulphanilamide |
| Molecular formula | C ₆ H ₈ N ₂ O ₂ S |
| Molar mass | 172,2 g/mol |
| CAS No | 63-74-1 |
| EC No | 200-563-4 |

SECTION 4: First aid measures

4.1 Description of first aid measures



General notes

Take off contaminated clothing.

Following inhalation

Provide fresh air.

Following skin contact

Rinse skin with water/shower.

Following eye contact

Rinse cautiously with water for several minutes.

Following ingestion

Rinse mouth. Call a doctor if you feel unwell.

4.2 Most important symptoms and effects, both acute and delayed

Symptoms and effects are not known to date.

4.3 Indication of any immediate medical attention and special treatment needed

none

SECTION 5: Firefighting measures

5.1 Extinguishing media



Safety data sheet

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



Sulphanilamide ROTI®CALIPURE 164-166 °C Melting point standard

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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_x), Carbon monoxide (CO), Carbon dioxide (CO₂), Sulphur oxides (SO_x)

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

No special measures are necessary.

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.

Other information relating to spills and releases

Place in appropriate containers for disposal. Ventilate affected area.

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

No special measures are necessary.

Advice on general occupational hygiene

Keep away from food, drink and animal feedingstuffs.

7.2 Conditions for safe storage, including any incompatibilities

Store in a dry place.

Safety data sheet

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



Sulphanilamide ROTI®CALIPURE 164-166 °C Melting point standard

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Incompatible substances or mixtures

Observe hints for combined storage.

Consideration of other advice:

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)

This information is not available.

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.

- **type of material**

NBR (Nitrile rubber)

- **material thickness**

>0,11 mm

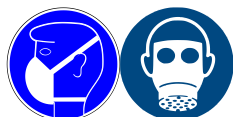
- **breakthrough times of the glove material**

>480 minutes (permeation: level 6)

- **other protection measures**

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

Respiratory protection



Safety data sheet

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



Sulphanilamide ROTI®CALIPURE 164-166 °C Melting point standard

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Respiratory protection necessary at: Dust formation. Particulate filter device (EN 143). P1 (filters at least 80 % 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 |
| Colour | whitish |
| Odour | characteristic |
| Melting point/freezing point | 163 – 167 °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 |
| Decomposition temperature | not relevant |
| pH (value) | 5,8 – 6,1 (in aqueous solution: 5 g/l, 20 °C) |
| Kinematic viscosity | not relevant |
| <u>Solubility(ies)</u> | |
| Water solubility | 7,5 g/l at 25 °C |
| <u>Partition coefficient</u> | |
| Partition coefficient n-octanol/water (log value): | -0,62 (Experimental data) |
| Vapour pressure | not determined |
| <u>Density and/or relative density</u> | |
| Density | 1,08 g/cm ³ |
| Relative vapour density | information on this property is not available |
| Bulk density | ~ 500 kg/m ³ |
| Particle characteristics | No data available. |
| <u>Other safety parameters</u> | |
| Oxidising properties | none |

Safety data sheet

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



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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

UV-radiation/sunlight.

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

Classification acc. to GHS

This substance does not meet the criteria for classification.

Acute toxicity

Shall not be classified as acutely toxic.

| Acute toxicity | | | | | |
|----------------|----------|-------------|---------|--------|--------|
| Exposure route | Endpoint | Value | Species | Method | Source |
| oral | LD50 | 3.900 mg/kg | rat | | TOXNET |

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.

Safety data sheet

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



Sulphanilamide ROTI®CALIPURE 164-166 °C Melting point standard

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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

Data are not available.

• If in eyes

Data are not available.

• If inhaled

Data are not available.

• If on skin

Data are not available.

• Other information

Health effects are not known. This information is based upon the present state of our knowledge.

11.2 Endocrine disrupting properties

Not listed.

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.

Biodegradation

Data are not available.

12.2 Process of degradability

Theoretical Oxygen Demand with nitrification: 1,695 mg/mg

Theoretical Oxygen Demand: 1,301 mg/mg

Theoretical Carbon Dioxide: 1,533 mg/mg

12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

| | |
|---------------------------|---------------------------|
| n-octanol/water (log KOW) | -0,62 (Experimental data) |
|---------------------------|---------------------------|

Safety data sheet

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



Sulphanilamide ROTI®CALIPURE 164-166 °C Melting point standard

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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



Consult the appropriate local waste disposal expert about waste disposal.

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).

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 <u>Information for each of the UN Model Regulations</u> | |
| 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. |

Safety data sheet

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



Sulphanilamide ROTI®CALIPURE 164-166 °C Melting point standard

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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)

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 % |
|-------------|-----|

Industrial Emissions Directive (IED)

| | |
|-------------|-----|
| VOC content | 0 % |
|-------------|-----|

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)

not listed

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

National regulations(GB)

List of substances subject to authorisation (GB REACH, Annex 14) / SVHC - candidate list

not listed

Restrictions according to GB REACH, Annex 17

not listed

Safety data sheet

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



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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 |
| TW | TCSI | substance is listed |
| US | TSCA | substance is listed |

Legend

| | |
|------------|---|
| AIIC | Australian Inventory of Industrial Chemicals |
| 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)

Alignment to regulation:

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): This substance does not meet the criteria for classification in accordance with Regulation No 1272/2008/EC. | Classification acc. to GHS: This substance does not meet the criteria for classification. | yes |
| 2.2 | Signal word: not required | | yes |

Safety data sheet

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



Sulphanilamide ROTI®CALIPURE 164-166 °C Melting point standard

article number: 9734

| Section | Former entry (text/value) | Actual entry (text/value) | Safety-relevant |
|---------|---|---|-----------------|
| 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 |

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) |
| CAS | Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances) |
| DGR | Dangerous Goods Regulations (see IATA/DGR) |
| 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) |
| EINECS | European Inventory of Existing Commercial Chemical Substances |
| ELINCS | European List of Notified Chemical Substances |
| GB REACH | The REACH etc. (Amendment etc.) (EU Exit) Regulations 2019, SI 2019/758 (as amended) |
| 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) |
| VOC | Volatile Organic Compounds |
| vPvB | Very Persistent and very Bioaccumulative |

Key literature references and sources for data

Agreement concerning the International Carriage of Dangerous Goods by Road (ADR). Regulations concerning the International Carriage of Dangerous Goods by Rail (RID). International Maritime Dangerous Goods Code (IMDG). Dangerous Goods Regulations (DGR) for the air transport (IATA).

Safety data sheet

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



Sulphanilamide ROTI®CALIPURE 164-166 °C Melting point standard

article number: **9734**

Disclaimer

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

Safety data sheet

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



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

article number: **9739**
Version: **4.0 en**
Replaces version of: 2020-10-27
Version: (3)

date of compilation: 2015-08-27
Revision: 2022-01-05

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 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 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
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

| 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)



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

article number: 9739

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 | Caffeine |
| Molecular formula | C ₈ H ₁₀ N ₄ O ₂ |
| Molar mass | 194,2 g/mol |
| CAS No | 58-08-2 |
| EC No | 200-362-1 |

Safety data sheet

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



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

article number: **9739**

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 |

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

Safety data sheet

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



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

article number: **9739**

In case of fire may be liberated: Nitrogen oxides (NO_x), Carbon monoxide (CO), Carbon dioxide (CO₂)

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.

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

Safety data sheet

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



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

article number: 9739

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 ³] | STEL [mg/m ³] | Ceiling-C [mg/m ³] | 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)

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 ³ | 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 | | | | |
|---|-----------------|-----------------------|------------------------------|------------------------------|
| Endpoint | 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

Safety data sheet

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



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

article number: 9739

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).

Environmental exposure controls

Keep away from drains, surface and ground water.

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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 |
| 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 ³ at 18 °C |
| Relative vapour density | information on this property is not available |
| Bulk density | 200 – 250 kg/m ³ |
| Particle characteristics | No data available. |
| <u>Other safety parameters</u> | |
| Oxidising properties | none |

9.2 Other information

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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.

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

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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

• 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

Not listed.

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 |

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

Biodegradation

The substance is readily biodegradable.

12.2 Process of degradability

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

Theoretical Oxygen Demand: 1,071 mg/mg

Theoretical Carbon Dioxide: 1,813 mg/mg

| 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) |
|---------------------------|-----------------------|

12.4 Mobility in soil

| | |
|--|--|
| Henry's law constant | 0 Pa m ³ /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

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.

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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).

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 | | |

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Deco-Paint Directive

| | |
|-------------|----------------|
| 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 |
| 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.

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National inventories

| Country | Inventory | 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 |

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)

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 |

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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) |
| 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 |
| 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 (http://www.nationalarchives.gov.uk/doc/open-government-licence/) |
| 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 |
| 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 |

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| Abbr. | Descriptions of used abbreviations |
|-------|--|
| TWA | Time-weighted average |
| VOC | Volatile Organic Compounds |
| vPvB | Very Persistent and very Bioaccumulative |
| WEL | Workplace exposure limit |

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.