

FLYLEAF

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	Num ber of piece s	Classification acc. to GHS	Pictograms	Page
Vanillin	CAS No 121-33-5 EC No 204-465-2 Article number 9714	1	Eye Irrit. 2A / H319	<u>(1)</u>	4 – 16
Sulphanilamide	CAS No 63-74-1 EC No 200-563-4 Article number 9734	1			17 – 27
Caffeine	CAS No 58-08-2 EC No 200-362-1 Article number 9739	1	Acute Tox. 4 / H302	<u>(1)</u>	28 – 40

Australia (en) Page 1 / 3



Article: 2921 Melting point standard Set 1 ROTI®Calipure

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

P270 Do not eat, drink or smoke when using this product

P280 Wear eye protection/face 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

P330 Rinse mouth

P337+P313 If eye irritation persists: Get medical advice/attention

Precautionary statements - disposal

P501 Dispose of contents/container to industrial combustion plant

3 Transport information

3.1 UN number not subject to transport regulations

3.2 UN proper shipping name not assigned
 3.3 Transport hazard class(es) not assigned
 3.4 Packing group not assigned

3.5 Environmental hazards non-environmentally hazardous acc. to the dan-

gerous goods regulations

3.6 Special precautions for user

There is no additional information.

3.7 Transport in bulk according to Annex II of MARPOL and the IBC Code

The cargo is not intended to be carried in bulk.

3.8 Information for each of the UN Model Regulations

Transport informationNational regulationsAdditional information(UN RTDG)

not assigned

Australia (en) Page 2 / 3



Article: 2921 Melting point standard Set 1 ROTI®Calipure

International Maritime Dangerous Goods Code (IMDG) - Additional information Not subject to IMDG.

International Civil Aviation Organization (ICAO-IATA/DGR) - Additional informationNot subject to ICAO-IATA.

Australia (en) Page 3 / 3

acc. to Safe Work Australia - Code of Practice

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

article number: 9714 date of compilation: 2019-04-29 Version: GHS 2.0 en Revision: 2022-05-16

Replaces version of: 2019-04-29

Version: (GHS 1)

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

Product identifier 1.1

Identification of the substance Vanillin ROTI®CALIPURE 81-83 °C Melting point

standard

9714 Article number

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 :Department Health, Safety and Environment

sheet:

e-mail (competent person): sicherheit@carlroth.de

1.4 **Emergency telephone number**

Name	Street	Postal code/city	Telephone	Website
NSW Poisons Information Centre Childrens Hospital	Hawkesbury Road	2145 West- mead, NSW	131126	

SECTION 2: Hazards identification

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	2A	Eye Irrit. 2A	H319

For full text of abbreviations: see SECTION 16

2.2 **Label elements**

Page 1 / 13 Australia (en)

acc. to Safe Work Australia - Code of Practice



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

article number: 9714

Labelling

Signal word Warning

Pictograms

GHS07



Hazard statements

H319 Causes serious eye irritation

Precautionary statements

Precautionary statements - prevention

P280 Wear eye protection/face 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 Call a POISON CENTER or doctor/physician if you feel unwell P312

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 $C_8H_8O_3$ 152.2 g/_{mol} Molar mass CAS No 121-33-5

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

Australia (en) Page 2 / 13

acc. to Safe Work Australia - Code of Practice

ROTH

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

article number: 9714

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.

6.3 Methods and material for containment and cleaning up

Advice on how to contain a spill

Covering of drains. Take up mechanically.

Australia (en) Page 3 / 13

acc. to Safe Work Australia - Code of Practice

ROTH

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

article number: 9714

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)

This information is not available.

Environmental values

Relevant PNECs and other threshold levels Threshold End-**Organism Environmental com-Exposure time** point level partment 0.118 ^{mg}/_I **PNEC** aquatic organisms freshwater short-term (single instance) **PNEC** 0.012 mg/_I aquatic organisms marine water short-term (single instance) **PNEC** 10 mg/_I aquatic organisms sewage treatment plant short-term (single instance)

(STP)

Australia (en) Page 4 / 13

acc. to Safe Work Australia - Code of Practice



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

article number: 9714

Relevant PNECs and other threshold levels

End- point	Threshold level	Organism	Environmental com- partment	Exposure time
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

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).

Australia (en) Page 5 / 13

acc. to Safe Work Australia - Code of Practice

ROTH

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

article number: 9714

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

Solubility(ies)

Water solubility $10^{9}/_{L}$ at 25 °C

Solubility in diethyl ether soluble
Solubility in ethyl acetate soluble

Partition coefficient

Partition coefficient n-octanol/water (log value): 1.17 – 1.21 (25 °C) (exp.)

Soil organic carbon/water (log KOC) 1.644 (ECHA)

Vapour pressure 0.0029 hPa at 25 °C

Density and/or relative density

Density $1.06 \, {}^{9}/_{cm^3}$ at 20 °C (ECHA)

Relative vapour density information on this property is not available

Bulk density $\sim 600 \, ^{\mathrm{kg}}/_{\mathrm{m}^3}$

Particle characteristics No data available.

Australia (en) Page 6 / 13

acc. to Safe Work Australia - Code of Practice



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

article number: 9714

Other safety parameters

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. Decompostion 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.

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.

Australia (en) Page 7 / 13

acc. to Safe Work Australia - Code of Practice

ROTH

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

article number: 9714

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.

SECTION 12: Ecological information

12.1 Toxicity

Harmful to aquatic life.

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	

Australia (en) Page 8 / 13

acc. to Safe Work Australia - Code of Practice



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

article number: 9714

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: $1.788 \frac{mg}{mg}$ /mg Theoretical Carbon Dioxide: $2.314 \frac{mg}{mg}$ /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.

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.

13.3 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.

Australia (en) Page 9 / 13

acc. to Safe Work Australia - Code of Practice



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

article number: 9714

SECTION 14: Transport information

14.1 UN number not subject to transport regulations

14.2 UN proper shipping name not assigned
 14.3 Transport hazard class(es) not assigned
 14.4 Packing group not assigned

14.5 Environmental hazards non-environmentally hazardous acc. to the dan-

gerous goods regulations

14.6 Special precautions for user

There is no additional information.

14.7 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 informationNational regulationsAdditional information(UN RTDG)

Not subject to transport regulations. UN RTDG

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 There is no additional information.

National regulations(Australia)

Australian Inventory of Chemical Substances(AICS)

Substance is listed.

Other information

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

National inventories

Country	Inventory	Status
AU	AIIC	substance is listed
CA	DSL	substance is listed
CN	IECSC	substance is listed
EU	ECSI	substance is listed
EU	REACH Reg.	substance is listed
JP	CSCL-ENCS	substance is listed
KR	KECI	substance is listed

Australia (en) Page 10 / 13

acc. to Safe Work Australia - Code of Practice



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

article number: 9714

Country	Inventory	Status
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 CICR CSCL-ENCS DSL ECSI Australian Inventory of Industrial Chemicals

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

INSQ 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

Taiwan Chemical Substance Inventory

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: Globally Harmonized System of Classification and Labelling of Chemicals ("Purple book").

Restructuring: section 9, section 14

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

Australia (en) Page 11 / 13

acc. to Safe Work Australia - Code of Practice



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

article number: 9714

Section	Former entry (text/value)	Actual entry (text/value)	Safety- relev- ant
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
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
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
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
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
UN RTDG	UN Recommendations on the Transport of Dangerous Good
vPvB	Very Persistent and very Bioaccumulative

Key literature references and sources for data

Safe Work Australia's Code of Practice for Labelling of Workplace Hazardous Chemicals (under WHS Regulations).

UN Recommendations on the Transport of Dangerous Good. 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.

Australia (en) Page 12 / 13

acc. to Safe Work Australia - Code of Practice



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

article number: 9714

Disclaimer

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

Australia (en) Page 13 / 13

acc. to Safe Work Australia - Code of Practice



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

article number: **9734**Version: **GHS 2.0 en**date of compilation: 2019-04-29
Revision: 2022-05-16

Replaces version of: 2019-04-29

Version: (GHS 1)

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
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 :Department Health, Safety and Environment

sheet:

e-mail (competent person): sicherheit@carlroth.de

1.4 Emergency telephone number

Name	Street	Postal code/city	Telephone	Website
NSW Poisons Information Centre Childrens Hospital	Hawkesbury Road	2145 West- mead, NSW	131126	

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

Australia (en) Page 1 / 11

acc. to Safe Work Australia - Code of Practice



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 $C_6H_8N_2O_2S$ Molar mass $172.2 \, {}^g/_{mol}$

CAS No 63-74-1

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



Suitable extinguishing media

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

Australia (en) Page 2 / 11

acc. to Safe Work Australia - Code of Practice



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

article number: 9734

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 (NOx), Carbon monoxide (CO), Carbon dioxide (CO₂), Sulphur oxides (SOx)

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.

Incompatible substances or mixtures

Observe hints for combined storage.

Australia (en) Page 3 / 11

acc. to Safe Work Australia - Code of Practice



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

article number: 9734

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





Respiratory protection necessary at: Dust formation. Particulate filter device (EN 143). P1 (filters at least 80 % of airborne particles, colour code: White).

Australia (en) Page 4 / 11

acc. to Safe Work Australia - Code of Practice



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

article number: 9734

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 not determined

range

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: $5 \frac{g}{l}$, 20 °C)

Kinematic viscosity not relevant

Solubility(ies)

Water solubility 7.5 9 / $_{1}$ at 25 $^{\circ}$ C

Partition coefficient

Partition coefficient n-octanol/water (log value): -0.62 (Experimental data)

Vapour pressure not determined

Density and/or relative density

Density $1.08 \, {}^{9}/_{cm^3}$

Relative vapour density information on this property is not available

Bulk density $\sim 500 \, \mathrm{kg}/\mathrm{m}^3$

Particle characteristics No data available.

Other safety parameters

Oxidising properties none

9.2 Other information

Australia (en) Page 5 / 11

acc. to Safe Work Australia - Code of Practice



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

article number: 9734

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.

Carcinogenicity

Shall not be classified as carcinogenic.

Australia (en) Page 6 / 11

acc. to Safe Work Australia - Code of Practice



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

article number: 9734

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.

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 $^{\rm mg}/_{\rm mg}$ Theoretical Oxygen Demand: 1.301 $^{\rm mg}/_{\rm mg}$ Theoretical Carbon Dioxide: 1.533 $^{\rm mg}/_{\rm mg}$

12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW)	-0.62 (Experimental data)
---------------------------	---------------------------

12.4 Mobility in soil

Data are not available.

12.5 Results of PBT and vPvB assessment

Data are not available.

Australia (en) Page 7 / 11

acc. to Safe Work Australia - Code of Practice



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

article number: 9734

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.

13.3 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 assigned
14.3	Transport hazard class(es)	not assigned
14.4	Packing group	not assigned

14.5 Environmental hazards non-environmentally hazardous acc. to the dan-

gerous goods regulations

14.6 Special precautions for user

There is no additional information.

14.7 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 informationNational regulationsAdditional information(UN RTDG)

Not subject to transport regulations. UN RTDG

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.

Australia (en) Page 8 / 11

acc. to Safe Work Australia - Code of Practice



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

article number: 9734

SECTION 15: Regulatory information

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

There is no additional information.

National regulations(Australia)

Australian Inventory of Chemical Substances(AICS)

Substance is listed.

Other information

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

National inventories

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

Legend

AIIC CSCL-ENCS DSL ECSI IECSC

Australian Inventory of Industrial Chemicals
List of Existing and New Chemical Substances (CSCL-ENCS)
Domestic Substances List (DSL)
EC Substance Inventory (EINECS, ELINCS, NLP)
Inventory of Existing Chemical Substances Produced or Imported in China
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

Toxic Substance Control Act

15.2 Chemical Safety Assessment

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

Australia (en) Page 9 / 11

acc. to Safe Work Australia - Code of Practice



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

article number: 9734

SECTION 16: Other information

Indication of changes (revised safety data sheet)

Alignment to regulation: Globally Harmonized System of Classification and Labelling of Chemicals

("Purple book").

Restructuring: section 9, section 14

Section	Former entry (text/value)	Actual entry (text/value)	Safety- relev- ant
2.1	Classification acc. to GHS	Classification acc. to GHS: This substance does not meet the criteria for classification.	yes
2.1		Classification acc. to GHS: change in the listing (table)	yes
2.2	Labelling GHS	Labelling: not required	yes
2.2	Signal word: Warning		yes
2.2	Hazard statements		yes
2.2		Hazard statements: change in the listing (table)	yes
2.2	Precautionary statements		yes
2.2	Precautionary statements - response		yes
2.2		Precautionary statements - response: change in the listing (table)	yes
2.2	Labelling of packages where the contents do not exceed 125 ml: Signal word: Warning		yes
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
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
DGR	Dangerous Goods Regulations (see IATA/DGR)
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
GHS	"Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Nations

Australia (en) Page 10 / 11

acc. to Safe Work Australia - Code of Practice



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

article number: 9734

Abbr.	Descriptions of used abbreviations
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
UN RTDG	UN Recommendations on the Transport of Dangerous Good
vPvB	Very Persistent and very Bioaccumulative

Key literature references and sources for data

Safe Work Australia's Code of Practice for Labelling of Workplace Hazardous Chemicals (under WHS Regulations).

UN Recommendations on the Transport of Dangerous Good. International Maritime Dangerous Goods Code (IMDG). Dangerous Goods Regulations (DGR) for the air transport (IATA).

Disclaimer

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

Australia (en) Page 11 / 11

acc. to Safe Work Australia - Code of Practice



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

article number: 9739 date of compilation: 2019-01-25 Version: GHS 3.0 en Revision: 2022-01-05

Replaces version of: 2020-10-27

Version: (GHS 2)

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

Product identifier 1.1

Identification of the substance Caffeine ROTI®CALIPURE anhydrous, Melting

point standard, 235-238 °C

Article number 9739 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 :Department Health, Safety and Environment

sheet:

e-mail (competent person): sicherheit@carlroth.de

1.4 **Emergency telephone number**

Name	Street	Postal code/city	Telephone	Website
NSW Poisons Information Centre Childrens Hospital	Hawkesbury Road	2145 West- mead, NSW	131126	

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
3.10	Acute toxicity (oral)	4	Acute Tox. 4	H302

For full text of abbreviations: see SECTION 16

2.2 **Label elements**

Page 1 / 13 Australia (en)

acc. to Safe Work Australia - Code of Practice



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

article number: 9739

Labelling

Signal word Warning

Pictograms

GHS07



Hazard statements

H302 Harmful if swallowed

Precautionary statements

Precautionary statements - prevention

P264 Wash thoroughly after handling

P270 Do not eat, drink or smoke when using this product

Precautionary statements - response

P301+P312 IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell

P330 Rinse mouth

Precautionary statements - disposal

P501 Dispose of contents/container to industrial combustion plant

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 $C_8H_{10}N_4O_2$ Molar mass 194.2 $^g/_{mol}$ CAS No 58-08-2

SECTION 4: First aid measures

4.1 Description of first aid measures



General notes

Take off contaminated clothing.

Following inhalation

Australia (en) Page 2 / 13

acc. to Safe Work Australia - Code of Practice

ROTH

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

article number: 9739

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

Following skin contact

Rinse skin with water/shower.

Following eye contact

Rinse cautiously with water for several minutes.

Following ingestion

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

4.2 Most important symptoms and effects, both acute and delayed

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

4.3 Indication of any immediate medical attention and special treatment needed

none

SECTION 5: Firefighting measures

5.1 Extinguishing media



Suitable extinguishing media

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

Unsuitable extinguishing media

water jet

5.2 Special hazards arising from the substance or mixture

Combustible.

Hazardous combustion products

In case of fire may be liberated: Nitrogen oxides (NOx), 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.

Australia (en) Page 3 / 13

acc. to Safe Work Australia - Code of Practice

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

article number: 9739

6.3 Methods and material for containment and cleaning up

Advice on how to contain a spill

Covering of drains. Take up mechanically.

Advice on how to clean up a spill

Take up mechanically. Control of dust.

Other information relating to spills and releases

Place in appropriate containers for disposal.

6.4 Reference to other sections

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

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Avoid dust formation.

Measures to prevent fire as well as aerosol and dust generation

Removal of dust deposits.

Advice on general occupational hygiene

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

7.2 Conditions for safe storage, including any incompatibilities

Store in a dry place.

Incompatible substances or mixtures

Observe hints for combined storage.

Consideration of other advice:

Ventilation requirements

Use local and general ventilation.

Specific designs for storage rooms or vessels

Recommended storage temperature: 15 - 25 °C

7.3 Specific end use(s)

No information available.

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.

Australia (en) Page 4 / 13

acc. to Safe Work Australia - Code of Practice



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

article number: 9739

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/m³	human, inhalatory	worker (industry)	chronic - systemic effects
DNEL	25.17 mg/kg bw/day	human, dermal	worker (industry)	chronic - systemic effects

Environmental values

Relevant PNECs and other threshold levels					
End- point	Threshold level	Organism	Environmental com- partment	Exposure time	
PNEC	0.087 ^{mg} / _l	aquatic organisms	freshwater	short-term (single instance)	
PNEC	0.009 ^{mg} / _l	aquatic organisms	marine water	short-term (single instance)	
PNEC	10 ^{mg} / _l	aquatic organisms	sewage treatment plant (STP)	short-term (single instance)	
PNEC	0.4 ^{mg} / _{kg}	aquatic organisms	freshwater sediment	short-term (single instance)	
PNEC	0.029 ^{mg} / _{kg}	terrestrial organisms	soil	short-term (single instance)	

8.2 Exposure controls

Individual protection measures (personal protective equipment)

Eye/face protection





Use safety goggle with side protection.

Skin protection





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)

Australia (en) Page 5 / 13

acc. to Safe Work Australia - Code of Practice



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

article number: 9739

material thickness

>0,11 mm

breakthrough times of the glove material

>480 minutes (permeation: level 6)

other protection measures

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

Respiratory protection





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

Environmental exposure controls

Keep away from drains, surface and ground water.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Physical state solid

Form powder, crystalline

Colour white
Odour odourless
Melting point/freezing point 236 – 239 °C
Boiling point or initial boiling point and boiling not determined

range

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: $10^{9}/_{1}$, 20° C)

Kinematic viscosity not relevant

Solubility(ies)

Water solubility 20 °C

Partition coefficient

Partition coefficient n-octanol/water (log value): -0.091 (23 °C) (ECHA)

Soil organic carbon/water (log KOC) 1 (ECHA)

Australia (en) Page 6 / 13

acc. to Safe Work Australia - Code of Practice



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

article number: 9739

Vapour pressure not determined

Density and/or relative density

Density $1.23 \, {}^{\rm g}/{}_{\rm cm^3}$ at 18 ${}^{\rm o}{\rm C}$

Relative vapour density information on this property is not available

Bulk density $200 - 250 \text{ kg/}_{\text{m}^3}$

Particle characteristics No data available.

Other safety parameters

Oxidising properties none

9.2 Other information

Information with regard to physical hazard hazard classes acc. to GHS

classes: (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

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

Classification acc. to GHS

Acute toxicity

Harmful if swallowed.

Australia (en) Page 7 / 13

acc. to Safe Work Australia - Code of Practice



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

article number: 9739

Acute toxicity					
Exposure route	Endpoint	Value	Species	Method	Source
oral	LD50	367.7 ^{mg} / _{kg}	rat		ECHA
dermal	LD50	>2,000 ^{mg} / _{kg}	rat		ECHA

Skin corrosion/irritation

Shall not be classified as corrosive/irritant to skin.

Serious eye damage/eye irritation

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

Respiratory or skin sensitisation

Shall not be classified as a respiratory or skin sensitiser.

Germ cell mutagenicity

Shall not be classified as germ cell mutagenic.

Carcinogenicity

Shall not be classified as carcinogenic.

Reproductive toxicity

Shall not be classified as a reproductive toxicant.

Specific target organ toxicity - single exposure

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

Specific target organ toxicity - repeated exposure

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

Aspiration hazard

Shall not be classified as presenting an aspiration hazard.

Symptoms related to the physical, chemical and toxicological characteristics

If swallowed

diarrhoea, vomiting

• If in eyes

essentially non-irritating

• 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.

Australia (en) Page 8 / 13

acc. to Safe Work Australia - Code of Practice



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

article number: 9739

SECTION 12: Ecological information

12.1 Toxicity

Harmful to aquatic life.

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

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 m³} / _{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.

Australia (en) Page 9 / 13

acc. to Safe Work Australia - Code of Practice



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

article number: 9739

12.7 Other adverse effects

Data are not available.

SECTION 13: Disposal considerations

13.1 Waste treatment methods



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

Sewage disposal-relevant information

Do not empty into drains.

13.3 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 assigned
14.3	Transport hazard class(es)	not assigned
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 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 informationNational regulationsAdditional information(UN RTDG)

Not subject to transport regulations. UN RTDG

International Maritime Dangerous Goods Code (IMDG) - Additional informationNot subject to IMDG.

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

Australia (en) Page 10 / 13

acc. to Safe Work Australia - Code of Practice



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

article number: 9739

SECTION 15: Regulatory information

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

There is no additional information.

National regulations(Australia)

Australian Inventory of Chemical Substances(AICS)

Substance is listed.

Other information

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

National inventories

Country	Inventory	Status
AU	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

Australian Inventory of Chemical Substances Chemical Inventory and Control Regulation List of Existing and New Chemical Substances (CSCL-ENCS) CSCL-ENCS DSL ECSI IECSC

Domestic Substances List (DSL)

EC Substance Inventory (EINECS, ELINCS, NLP)
Inventory of Existing Chemical Substances Produced or Imported in China National Inventory of Chemical Substances

Korea Existing Chemicals Inventory
New Zealand Inventory of Chemicals
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.

Australia (en) Page 11 / 13

acc. to Safe Work Australia - Code of Practice



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

article number: 9739

SECTION 16: Other information

Indication of changes (revised safety data sheet)

Alignment to regulation: Globally Harmonized System of Classification and Labelling of Chemicals ("Purple book").

Restructuring: section 9, section 14

Section	Former entry (text/value)	Actual entry (text/value)	Safety- relev- ant
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
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
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
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
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
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

Australia (en) Page 12 / 13

acc. to Safe Work Australia - Code of Practice



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

article number: 9739

Abbr.	Descriptions of used abbreviations
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
UN RTDG	UN Recommendations on the Transport of Dangerous Good
vPvB	Very Persistent and very Bioaccumulative

Key literature references and sources for data

Safe Work Australia's Code of Practice for Labelling of Workplace Hazardous Chemicals (under WHS Regulations).

UN Recommendations on the Transport of Dangerous Good. 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.

Australia (en) Page 13 / 13