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



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

article number: 9739 date of compilation: 2015-08-27 Version: **5.0 en** Revision: 2024-03-04

Replaces version of: 2022-01-05

Version: (4)

# 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

Index No (GB CLP) 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

Laboratory chemical Relevant identified uses:

Laboratory and analytical use

Uses advised against: Do not use for private purposes (household).

Food, drink and animal feedingstuffs.

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

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

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

sheet:

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

#### **Emergency telephone number** 1.4

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

For full text of abbreviations: see SECTION 16

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#### 2.2 Label elements

Labelling

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

# 2.3 Other hazards

# Results of PBT and vPvB assessment

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

# **Endocrine disrupting properties**

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

# **SECTION 3: Composition/information on ingredients**

# 3.1 Substances

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

# Substance, Specific Conc. Limits, M-factors, ATE

Specific Conc. Limits	M-Factors	ATE	Exposure route
-	-	367,7 <sup>mg</sup> / <sub>kg</sub>	oral

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# **SECTION 4: First aid measures**

# 4.1 Description of first aid measures



#### **General notes**

Take off contaminated clothing.

# Following inhalation

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

# **Following skin contact**

Rinse skin with water/shower.

# Following eye contact

Rinse cautiously with water for several minutes.

# **Following ingestion**

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

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

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

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

none

# **SECTION 5: Firefighting measures**

# 5.1 Extinguishing media



# Suitable extinguishing media

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

# Unsuitable extinguishing media

water jet

# 5.2 Special hazards arising from the substance or mixture

Combustible.

# **Hazardous combustion products**

In case of fire may be liberated: Nitrogen oxides (NOx), Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>)

# 5.3 Advice for firefighters

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

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# **SECTION 6: Accidental release measures**

# 6.1 Personal precautions, protective equipment and emergency procedures



# For non-emergency personnel

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

# 6.2 Environmental precautions

Keep away from drains, surface and ground water. Retain contaminated washing water and dispose of it.

# 6.3 Methods and material for containment and cleaning up

# Advice on how to contain a spill

Covering of drains. Take up mechanically.

# Advice on how to clean up a spill

Take up mechanically. Control of dust.

# Other information relating to spills and releases

Place in appropriate containers for disposal.

#### 6.4 Reference to other sections

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

# **SECTION 7: Handling and storage**

# 7.1 Precautions for safe handling

Avoid dust formation.

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

Removal of dust deposits.

# Advice on general occupational hygiene

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

# 7.2 Conditions for safe storage, including any incompatibilities

Store in a dry place.

# **Incompatible substances or mixtures**

Observe hints for combined storage.

# Consideration of other advice:

# **Ventilation requirements**

Use local and general ventilation.

# Specific designs for storage rooms or vessels

Recommended storage temperature: 15 - 25 °C

# 7.3 Specific end use(s)

No information available.

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# SECTION 8: Exposure controls/personal protection

# **Control parameters**

# **National limit values**

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

Coun	Name of agent	CAS No	Identifi- er	TWA [mg/ m³]	STEL [mg/ m³]	Ceil- ing-C [mg/ m³]	Nota- tion	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

Inhalable fraction Respirable fraction

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) **STEL** 

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

#### **Environmental values**

#### Relevant PNECs and other threshold levels End-**Threshold Organism Environmental com-Exposure time** point level partment **PNEC** 0,087 mg/I freshwater aquatic organisms short-term (single instance) **PNEC** 0,009 mg/I aquatic organisms marine water short-term (single instance) **PNEC** 10 mg/i aquatic organisms sewage treatment plant short-term (single instance) (STP) $0.4 \, \text{mg}/\text{kg}$ **PNEC** freshwater sediment aquatic organisms short-term (single instance) 0,029 mg/kg **PNEC** terrestrial organisms soil short-term (single instance)

#### 8.2 **Exposure controls**

Individual protection measures (personal protective equipment)

**Eye/face protection** 



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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.

# 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

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# ROTH

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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:  $10 \, {}^{9}/_{l}$ ,  $20 \, {}^{\circ}$ 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)

Vapour pressure not determined

Density and/or relative density

Density 1,23 <sup>g</sup>/<sub>cm³</sub> at 18 °C

Relative vapour density Information on this property is not available.

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

Particle characteristics No data available.

Other safety parameters

Oxidising properties none

9.2 Other information

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

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# 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.

GHS of the United Nations, annex 4. May be harmful in contact with skin.

Acute toxicity					
Exposure route	Endpoint	Value	Species	Method	Source
oral	LD50	367,7 <sup>mg</sup> / <sub>kg</sub>	rat		ECHA
dermal	LD50	>2.000 <sup>mg</sup> / <sub>kg</sub>	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.

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# 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

Does not contain an endocrine disruptor (ED) at a concentration of  $\geq 0.1\%$ .

#### 11.3 Information on other hazards

There is no additional information.

# **SECTION 12: Ecological information**

# 12.1 Toxicity

Shall not be classified as hazardous to the aquatic environment.

Aquatic toxicity (acute)					
Endpoint	Value	Species	Source	Exposure time	
LC50	87 <sup>mg</sup> / <sub>l</sub>	fish	ECHA	96 h	
EC50	182 <sup>mg</sup> / <sub>l</sub>	aquatic invertebrates	ECHA	48 h	
ErC50	>100 <sup>mg</sup> / <sub>I</sub>	algae	ECHA	72 h	

# Aquatic toxicity (chronic) Endpoint Value Species Source Exposure time EC50 3.490 mg/<sub>I</sub> microorganisms ECHA 17 h

# 12.2 Persistence and degradability

Theoretical Oxygen Demand (without nitrification): 1,071  $^{\rm mg}/_{\rm mg}$  Theoretical Oxygen Demand (with nitrification): 1,617  $^{\rm mg}/_{\rm mg}$  Theoretical Carbon Dioxide: 1,813  $^{\rm mg}/_{\rm mg}$ 

# **Biodegradation**

The substance is readily biodegradable.

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# **Process of degradability**

Process	Degradation rate	Time
biotic/abiotic	90 – 100 %	22 d
DOC removal	>90 – 100 %	22 d

# 12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

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

Henry's law constant	0 <sup>Pa m³</sup> / <sub>mol</sub> at 25 °C (ECHA)
The Organic Carbon normalised adsorption coefficient	1 (ECHA)

#### 12.5 Results of PBT and vPvB assessment

Data are not available.

# 12.6 Endocrine disrupting properties

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

#### 12.7 Other adverse effects

Data are not available.

# **SECTION 13: Disposal considerations**

#### 13.1 Waste treatment methods



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

# Sewage disposal-relevant information

Do not empty into drains.

# Waste treatment of containers/packagings

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

# 13.2 Relevant provisions relating to waste

The allocation of waste identity numbers/waste descriptions must be carried out according to the EEC, specific to the industry and process.

# Properties of waste which render it hazardous

**HP 6** acute toxicity

#### 13.3 Remarks

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

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# **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 dan-

gerous 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

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)

# **Seveso Directive**

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

# **Deco-Paint Directive**

VOC content	0 %
VOC content	0 <sup>g</sup> / <sub>l</sub>

# **Industrial Emissions Directive (IED)**

VOC content	0 %
VOC content	0 <sup>g</sup> / <sub>l</sub>

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

not listed

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# 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 pos- sess 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

#### 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

#### 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

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Country	Inventory	Status
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 (ACTIVE)
VN	NCI	substance is listed

Legend

Australian Inventory of Industrial Chemicals Chemical Inventory and Control Regulation List of Existing and New Chemical Substances (CSCL-ENCS) AIIC CICR 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 INSQ

NCI National Chemical Inventory
NZIOC New Zealand Inventory of Chemicals
PICCS Philippine Inventory of Chemicals and Chemical Substances (PICCS)
REACH Reg. REACH registered substances
TCSI Taiwan Chemical Substance Inventory

TSCA Toxic Substance Control Act

# 15.2 Chemical safety assessment

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

# **SECTION 16: Other information**

# Indication of changes (revised safety data sheet)

Section	Former entry (text/value)	Actual entry (text/value)	Safety- relev- ant
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		Endocrine disrupting properties: Does not contain an endocrine disruptor (ED) at a concentration of ≥ 0,1%.	yes
14.8	Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN) - Additional information:  Not subject to ADR, RID and ADN.		yes
15.1	Restrictions according to REACH, Annex XVII: not listed		yes

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Section	Former entry (text/value)	Actual entry (text/value)	Safety- relev- ant
15.1	List of substances subject to authorisation (REACH, Annex XIV)/SVHC - candidate list: Not listed.		yes
15.1	VOC content: 0 % , 0 <sup>g</sup> / <sub>l</sub>	VOC content: 0 %	yes
15.1		VOC content: 0 <sup>g</sup> / <sub>l</sub>	yes
15.1		National regulations(GB)	yes
15.1		List of substances subject to authorisation (GB REACH, Annex 14) / SVHC - candidate list: not listed	yes
15.1		Restrictions according to GB REACH, Annex 17: not listed	yes
15.1		National inventories: change in the listing (table)	yes

# **Abbreviations and acronyms**

Abbr.	Descriptions of used abbreviations	
ADR	Accord relatif au transport international des marchandises dangereuses par route (Agreement concerning the International Carriage of Dangerous Goods by Road)	
ATE	Acute Toxicity Estimate	
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)	
Ceiling-C	Ceiling value	
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)	
ED	Endocrine disruptor	
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 CLP	The Chemicals (Health and Safety) and Genetically Modified Organisms (Contained Use) (Amendment etc.) (EU Exit) Regulations 2019, SI 2019/720 (as amended)	
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	

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Abbr.	Descriptions of used abbreviations
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
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
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.

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