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

β-Ionone pure

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

Product identifier 1.1

Identification of the substance **β-Ionone** pure

Article number 3951

It is not required to list the identified uses be-Registration number (REACH)

cause the substance is not subject to registration

according to REACH (< 1 t/a).

EC number 201-224-3 CAS number 79-77-6

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:

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

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

Section	Hazard class	Cat- egory	Hazard class and category	Hazard statement
4.1C	Hazardous to the aquatic environment - chronic hazard	2	Aquatic Chronic 2	H411

For full text of abbreviations: see SECTION 16

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The most important adverse physicochemical, human health and environmental effects Spillage and fire water can cause pollution of watercourses.

2.2 Label elements

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

Signal word Not required

Pictograms

GHS09



Hazard statements

H411 Toxic to aquatic life with long lasting effects

Precautionary statements

Precautionary statements - prevention

P273 Avoid release to the environment

Labelling of packages where the contents do not exceed 125 ml

Signal word: Not required.

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 β -Ionone Molecular formula $C_{13}H_{20}O$ Molar mass $192,3\,^9/_{mol}$ CAS No 79-77-6 EC No 201-224-3

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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.

Following skin contact

Wash with plenty of soap and water.

Following eye contact

Irrigate copiously with clean, fresh water, holding the eyelids apart.

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 spray, dry extinguishing powder, BC-powder, carbon dioxide (CO₂)

Unsuitable extinguishing media

water jet

5.2 Special hazards arising from the substance or mixture

Combustible.

Hazardous combustion products

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

5.3 Advice for firefighters

In case of fire and/or explosion do not breathe fumes. Do not allow firefighting water to enter drains or water courses. 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

Wearing of suitable protective equipment (including personal protective equipment referred to under Section 8 of the safety data sheet) to prevent any contamination of skin, eyes and personal clothing. Avoid contact with skin, eyes and clothes. Do not breathe vapour/spray.

6.2 Environmental precautions

Keep away from drains, surface and ground water. Retain contaminated washing water and dispose of it. If substance has entered a water course or sewer, inform the responsible authority.

6.3 Methods and material for containment and cleaning up

Advice on how to contain a spill

Covering of drains.

Advice on how to clean up a spill

Absorb with liquid-binding material (sand, diatomaceous earth, acid- or universal binding agents).

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.

Measures to protect the environment

Avoid release to the environment.

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

Keep in a cool place.

Incompatible substances or mixtures

Observe hints for combined storage.

Consideration of other advice:

Specific designs for storage rooms or vessels

Recommended storage temperature: 2 - 8 °C

7.3 Specific end use(s)

No information available.

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SECTION 8: Exposure controls/personal protection

8.1 Control parameters

National limit values

Occupational exposure limit values (Workplace Exposure Limits)

Data are not available.

Human health values

Relevant DNELs and other threshold levels						
Endpoint	Threshold level	Protection goal, route of exposure	Used in	Exposure time		
DNEL	12,7 mg/m ³	human, inhalatory	worker (industry)	chronic - systemic effects		
DNEL	6 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	0,004 ^{mg} / _l	aquatic organisms	freshwater	short-term (single instance)		
PNEC	0 ^{mg} / _l	aquatic organisms	marine water	short-term (single instance)		
PNEC	1 ^{mg} / _l	aquatic organisms	sewage treatment plant (STP)	short-term (single instance)		
PNEC	0,151 ^{mg} / _{kg}	aquatic organisms	freshwater sediment	short-term (single instance)		
PNEC	0,015 ^{mg} / _{kg}	aquatic organisms	marine sediment	short-term (single instance)		
PNEC	0,051 ^{mg} / _{kg}	terrestrial organisms	soil	short-term (single instance)		

8.2 Exposure controls

Individual protection measures (personal protective equipment)

Eye/face protection





Use safety goggle with side protection.

Skin protection





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hand protection

Wear suitable gloves. Chemical protection gloves are suitable, which are tested according to EN 374. For special purposes, it is recommended to check the resistance to chemicals of the protective gloves mentioned above together with the supplier of these gloves. The times are approximate values from measurements at 22 ° C and permanent contact. Increased temperatures due to heated substances, body heat etc. and a reduction of the effective layer thickness by stretching can lead to a considerable reduction of the breakthrough time. If in doubt, contact manufacturer. At an approx. 1.5 times larger / smaller layer thickness, the respective breakthrough time is doubled / halved. The data apply only to the pure substance. When transferred to substance mixtures, they may only be considered as a guide.

type of material

NBR (Nitrile rubber)

material thickness

0,7mm

breakthrough times of the glove material

>10 minutes (permeation: level 1)

other protection measures

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

Respiratory protection





Respiratory protection necessary at: Aerosol or mist formation. Type: A (against organic gases and vapours with a boiling point of > 65 °C , colour code: Brown).

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 liquid

Colour light yellow
Odour characteristic

Melting point/freezing point -35 °C

Boiling point or initial boiling point and boiling 267,1 °C at 1.013 hPa (ECHA)

range

Flammability this material is combustible, but will not ignite

readily

Lower and upper explosion limit not determined

Flash point 126 °C at 1.013 hPa (ECHA) Auto-ignition temperature 273 °C at 1.017 hPa (ECHA)

Decomposition temperature not relevant pH (value) not determined

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Kinematic viscosity 11,8 ^{mm²}/_s at 20 °C

Solubility(ies)

Water solubility $0,11 \text{ g/}_{1}$ at 20 °C (ECHA)

Partition coefficient

Partition coefficient n-octanol/water (log value): 4 (25 °C) (ECHA)

Soil organic carbon/water (log KOC) 2,8 (ECHA)

Vapour pressure 0,072 hPa at 25 °C

Density $0.945 \, {}^{9}/_{cm^3}$ at 20 ${}^{\circ}\text{C}$

Relative vapour density information on this property is not available

Particle characteristics not relevant (liquid)

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:

Refractive index 1,519

Temperature class (EU, acc. to ATEX) T3

Maximum permissible surface temperature on

the equipment: 200°C

SECTION 10: Stability and reactivity

10.1 Reactivity

This material is not reactive under normal ambient conditions.

If heated

Vapours may form explosive mixtures with air.

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

There are no specific conditions known which have to be avoided.

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10.5 Incompatible materials

oxidisers

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

Shall not be classified as acutely toxic.

Acute toxicity						
Exposure route	Endpoint	Value	Species	Method	Source	
oral	LD50	2.920 ^{mg} / _{kg}	rat			
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

Data are not available.

• If in eyes

Data are not available.

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If inhaled

Data are not available.

• If on skin

Data are not available.

Other information

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

Toxic to aquatic life with long lasting effects.

Aquatic toxicity (acute)						
Endpoint	Value	Species	Source	Exposure time		
LC50	5,09 ^{mg} / _l	fish	ECHA	96 h		
EC50	4,71 ^{mg} / _l	fish	ECHA	96 h		
ErC50	22,15 ^{mg} / _l	algae	ECHA	72 h		

Aquatic toxicity (chronic)

Endpoint	Value	Species	Source	Exposure time
EC50	200 ^{mg} / _l	microorganisms	ECHA	180 min

Biodegradation

The substance is readily biodegradable.

12.2 Process of degradability

Theoretical Oxygen Demand: $2,912 \frac{mg}{mg}$ Theoretical Carbon Dioxide: $2,975 \frac{mg}{mg}$

Process of degradability

Process	Degradation rate	Time
oxygen depletion	70 – 80 %	28 d

12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

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n-octanol/water (log KOW)	4 (25 °C) (ECHA)
BCF	202,4 (ECHA)

12.4 Mobility in soil

The Organic Carbon normalised adsorption coefficient	2,8 (ECHA)
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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. Avoid release to the environment. Refer to special instructions/safety data sheets.

Waste treatment of containers/packagings

It is a dangerous waste; only packagings which are approved (e.g. acc. to ADR) may be used.

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

ADR/RID/ADN UN 3082
IMDG-Code UN 3082
ICAO-TI UN 3082

14.2 UN proper shipping name

ADR/RID/ADN ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LI-QUID, N.O.S.

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IMDG-Code ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LI-

QUID, N.O.S.

ICAO-TI Environmentally hazardous substance, liquid,

n.o.s.

Technical name β-Ionone

14.3 Transport hazard class(es)

ADR/RID/ADN 9
IMDG-Code 9
ICAO-TI 9

14.4 Packing group

ADR/RID/ADN III
IMDG-Code III
ICAO-TI III

14.5 Environmental hazards hazardous to the aquatic environment

14.6 Special precautions for user

Provisions for dangerous goods (ADR) should be complied within the premises.

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

Proper shipping name ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LI-

QUID, N.O.S.

Particulars in the transport document UN3082, ENVIRONMENTALLY HAZARDOUS SUB-

STANCE, LIQUID, N.O.S., (β-Ionone), 9, III, (-)

Classification code M6

Danger label(s) 9, "Fish and tree"

M



Environmental hazards yes (hazardous to the aquatic environment)

Special provisions (SP) 274, 335, 375, 601

Excepted quantities (EQ) E1
Limited quantities (LQ) 5 L
Transport category (TC) 3
Tunnel restriction code (TRC) Hazard identification No 90

Emergency Action Code 3Z

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International Maritime Dangerous Goods Code (IMDG) - Additional information

Proper shipping name ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LI-

QUID, N.O.S.

Particulars in the shipper's declaration UN3082, ENVIRONMENTALLY HAZARDOUS SUB-

STANCE, LIQUID, N.O.S., (β-Ionone), 9, III

Marine pollutant **yes** (hazardous to the aquatic environment), (β-Ionone)

Danger label(s) 9. "Fish and tree"

Special provisions (SP) 274, 335, 969

Excepted quantities (EQ) E1 Limited quantities (LQ) 5 L

F-A, S-F **EmS**

Stowage category Α

International Civil Aviation Organization (ICAO-IATA/DGR) - Additional information

Proper shipping name Environmentally hazardous substance, liquid,

Particulars in the shipper's declaration UN3082, Environmentally hazardous substance,

liquid, n.o.s., (β-Ionone), 9, III

Environmental hazards YES (hazardous to the aquatic environment)

Danger label(s) 9, "Fish and tree"

Special provisions (SP) A97, A158, A197, A215

Excepted quantities (EQ) E1 Limited quantities (LQ) 30 kg

SECTION 15: Regulatory information

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

Dangerous substances with restrictions (REACH, Annex XVII)

Name of substance	Name acc. to inventory	CAS No	Restriction	No
β-Ionone	this product meets the criteria for classification in accordance with Reg- ulation No 1272/2008/EC		R3	З

Legend

1. Shall not be used in:

- ornamental articles intended to produce light or colour effects by means of different phases, for example in ornamental lamps and ashtrays,

tricks and jokes,

- games for one or more participants, or any article intended to be used as such, even with ornamental aspects, 2. Articles not complying with paragraph 1 shall not be placed on the market.

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Legend

3. Shall not be placed on the market if they contain a colouring agent, unless required for fiscal reasons, or perfume, or both, if they

can be used as fuel in decorative oil lamps for supply to the general public, and

present an aspiration hazard and are labelled with H304.
 Decorative oil lamps for supply to the general public shall not be placed on the market unless they conform to the European Standard on Decorative oil lamps (EN 14059) adopted by the European Committee for Standardisation

(CEN).
5. Without prejudice to the implementation of other Union provisions relating to the classification, labelling and packaging of substances and mixtures, suppliers shall ensure, before the placing on the market, that the following require-

(a) lamp oils, labelled with H304, intended for supply to the general public are visibly, legibly and indelibly marked as follows: "Keep lamps filled with this liquid out of the reach of children"; and, by 1 December 2010, "Just a sip of lamp oil – or even sucking the wick of lamps – may lead to life-threatening lung damage"; (b) grill lighter fluids, labelled with H304, intended for supply to the general public are legibly and indelibly marked by 1 December 2010 as follows: "Just a sip of grill lighter fluid may lead to life threatening lung damage"; (c) lamps oils and grill lighters, labelled with H304, intended for supply to the general public are packaged in black on acquire containers not exceeding 1 litre by 1 December 2010."

opaque containers not exceeding 1 litre by 1 December 2010.';

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

Not listed.

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				
E2	environmental hazards (hazardous to the aquatic environment, cat. 2)	200 500	57)				

Notation

Hazardous to the Aquatic Environment in category Chronic 2

Deco-Paint Directive

VOC content 0 % 0 9/	
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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)

not listed

Regulation on the marketing and use of explosives precursors

not listed

Regulation on drug precursors

not listed

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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 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
NZ	NZIoC	substance is listed
PH	PICCS	substance is listed
TW	TCSI	substance is listed
US	TSCA	substance is listed

Legend

AICS Australian Inventory of Chemical Substances
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 KECI Korea Existing Chemicals Inventory

New Zealand Inventory of Chemicals 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

Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
ADN	Accord européen relatif au transport international des marchandises dangereuses par voies de naviga- tion intérieures (European Agreement concerning the International Carriage of Dangerous Goods by In- land Waterways)
ADR	Accord relatif au transport international des marchandises dangereuses par route (Agreement concerning the International Carriage of Dangerous Goods by Road)
ADR/RID/ADN	Agreements concerning the International Carriage of Dangerous Goods by Road/Rail/Inland Waterways (ADR/RID/ADN)
BCF	Bioconcentration factor

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Abbr.	Descriptions of used abbreviations
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
CLP	Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures
DGR	Dangerous Goods Regulations (see IATA/DGR)
DNEL	Derived No-Effect Level
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)
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
EmS	Emergency Schedule
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
ICAO-TI	Technical instructions for the safe transport of dangerous goods by air
IMDG	International Maritime Dangerous Goods Code
IMDG-Code	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
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RID	Règlement concernant le transport International ferroviaire des marchandises Dangereuses (Regulations concerning the International carriage of Dangerous goods by Rail)
SVHC	Substance of Very High Concern
VOC	Volatile Organic Compounds
vPvB	Very Persistent and very Bioaccumulative

Key literature references and sources for data

Regulation (EC) No 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).

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

Code	Text
H411	Toxic to aquatic life with long lasting effects.

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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