

# Voluntary safety information following the Safety Data Sheet format according to Regulation (EC) No. 1907/2006 (REACH)



## $\alpha$ -Ionone pure

article number: 3950  
Version: 1.0 en

date of compilation: 2021-07-08

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

### 1.1 Product identifier

Identification of the substance	$\alpha$ -Ionone pure
Article number	3950
EC number	204-841-6
CAS number	127-41-3

### 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

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Competent person responsible for the safety data sheet: Department Health, Safety and Environment

**e-mail (competent person):** [sicherheit@carlroth.de](mailto:sicherheit@carlroth.de)

### 1.4 Emergency telephone number

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

## SECTION 2: Hazards identification

### 2.1 Classification of the substance or mixture

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

This substance does not meet the criteria for classification in accordance with Regulation No 1272/2008/EC.

### 2.2 Label elements

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

not required

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### 2.3 Other hazards

This material is combustible, but will not ignite readily.

#### 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	$\alpha$ -Ionone
Molecular formula	C <sub>13</sub> H <sub>20</sub> O
Molar mass	192,3 g/mol
CAS No	127-41-3
EC No	204-841-6

## 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

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## 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 (CO<sub>2</sub>)

#### 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 (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.

## 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.

#### 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.

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## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

Provision of sufficient ventilation.

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



Keep away from sources of ignition - No smoking.

**Advice on general occupational hygiene**

Keep away from food, drink and animal feedingstuffs.

### 7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed.

**Incompatible substances or mixtures**

Observe hints for combined storage.

**Consideration of other advice:**

**Specific designs for storage rooms or vessels**

Recommended storage temperature: 15 – 25 °C

### 7.3 Specific end use(s)

No information available.

## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

**National limit values**

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

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	0,987 mg/m <sup>3</sup>	human, inhalatory	worker (industry)	chronic - systemic effects
DNEL	0,28 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 compartment	Exposure time
PNEC	3,4 µg/l	aquatic organisms	freshwater	short-term (single instance)
PNEC	0,34 µg/l	aquatic organisms	marine water	short-term (single instance)

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Relevant PNECs and other threshold levels				
End-point	Threshold level	Organism	Environmental compartment	Exposure time
PNEC	13,1 mg/l	aquatic organisms	sewage treatment plant (STP)	short-term (single instance)
PNEC	0,984 mg/kg	aquatic organisms	freshwater sediment	short-term (single instance)
PNEC	98,4 µg/kg	aquatic organisms	marine sediment	short-term (single instance)
PNEC	0,195 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.

**• 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: 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.

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**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	<-15,6 °C at 965,7 hPa (ECHA)
Boiling point or initial boiling point and boiling range	207,7 °C at 968,6 hPa (ECHA)
Flammability	this material is combustible, but will not ignite readily
Lower and upper explosion limit	not determined
Flash point	87,3 °C at 973 hPa (ECHA)
Auto-ignition temperature	not determined
Decomposition temperature	not relevant
pH (value)	not determined
Kinematic viscosity	41,15 mm <sup>2</sup> /s at 20 °C
<u>Solubility(ies)</u>	
Water solubility	0,05871 g/l at 25 °C
<u>Partition coefficient</u>	
Partition coefficient n-octanol/water (log value):	3,896 (pH value: 7,2, 25 °C) (ECHA)
Soil organic carbon/water (log KOC)	3,456 (ECHA)

Vapour pressure 0,0361 hPa at 25 °C

Density 0,922 g/cm<sup>3</sup> at 20 °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 classes: hazard classes acc. to GHS (physical hazards): not relevant

Other safety characteristics:

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Surface tension

22,33 mN/m (124 °C) (ECHA)

## 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.

### 10.5 Incompatible materials

There is no additional information.

### 10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.

## SECTION 11: Toxicological information

### 11.1 Information on hazard classes as defined in Regulation (EC) No 1272/2008

#### Classification according to GHS (1272/2008/EC, CLP)

This substance does not meet the criteria for classification in accordance with Regulation No 1272/2008/EC.

#### Acute toxicity

Shall not be classified as acutely toxic.

Acute toxicity					
Exposure route	Endpoint	Value	Species	Method	Source
oral	LD50	4.590 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.

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**Carcinogenicity**

Shall not be classified as carcinogenic.

**Reproductive toxicity**

Shall not be classified as a reproductive toxicant.

**Specific target organ toxicity - single exposure**

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

**Specific target organ toxicity - repeated exposure**

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

**Aspiration hazard**

Shall not be classified as presenting an aspiration hazard.

**Symptoms related to the physical, chemical and toxicological characteristics**

• **If swallowed**

Data are not available.

• **If in eyes**

Data are not available.

• **If inhaled**

Data are not available.

• **If on skin**

Data are not available.

• **Other information**

Health effects are not known.

**11.2 Endocrine disrupting properties**

Not listed.

**11.3 Information on other hazards**

There is no additional information.

**SECTION 12: Ecological information**

**12.1 Toxicity**

Shall not be classified as hazardous to the aquatic environment.

**Biodegradation**

Data are not available.

**12.2 Process of degradability**

Theoretical Oxygen Demand: 2,912 mg/mg  
Theoretical Carbon Dioxide: 2,975 mg/mg

Process of degradability		
Process	Degradation rate	Time
oxygen depletion	41,92 %	42 d



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**12.3 Bioaccumulative potential**

Does not significantly accumulate in organisms.

n-octanol/water (log KOW)	3,896 (pH value: 7,2, 25 °C) (ECHA)
BCF	161 (ECHA)

**12.4 Mobility in soil**

The Organic Carbon normalised adsorption coefficient	3,456 (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**



Consult the appropriate local waste disposal expert about waste disposal.

**Sewage disposal-relevant information**

Do not empty into drains.

**13.2 Relevant provisions relating to waste**

The allocation of waste identity numbers/waste descriptions must be carried out according to the EEC, specific to the industry and process. Waste catalogue ordinance (Germany).

**13.3 Remarks**

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

**SECTION 14: Transport information**

- |  |   |
|--|---|
| <b>14.1 UN number or ID number</b>       | not subject to transport regulations                                  |
| <b>14.2 UN proper shipping name</b>      | not assigned  |
| <b>14.3 Transport hazard class(es)</b>   | none  |
| <b>14.4 Packing group</b>                | not assigned  |
| <b>14.5 Environmental hazards</b>        | non-environmentally hazardous acc. to the dangerous goods regulations |
| <b>14.6 Special precautions for user</b> | There is no additional information.                                   |

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**14.7 Maritime transport in bulk according to IMO instruments**

The cargo is not intended to be carried in bulk.

**14.8 Information for each of the UN Model Regulations**

**Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN) - Additional information**

Not subject to ADR, RID and ADN.

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

Not subject to IMDG.

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

Not subject to ICAO-IATA.

**SECTION 15: Regulatory information**

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

**Relevant provisions of the European Union (EU)**

**Restrictions according to REACH, Annex XVII**

not listed

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

Not listed.

**Seveso Directive**

**2012/18/EU (Seveso III)**

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

**Deco-Paint Directive**

VOC content	100 % 922 g/l
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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

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### 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 inventories

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

#### Legend

AICS	Australian Inventory of Chemical Substances
CICR	Chemical Inventory and Control Regulation
CSCL-ENCS	List of Existing and New Chemical Substances (CSCL-ENCS)
DSL	Domestic Substances List (DSL)
ECSI	EC Substance Inventory (EINECS, ELINCS, NLP)
IECSC	Inventory of Existing Chemical Substances Produced or Imported in China
INSQ	National Inventory of Chemical Substances
KECI	Korea Existing Chemicals Inventory
NZIoC	New Zealand Inventory of Chemicals
PICCS	Philippine Inventory of Chemicals and Chemical Substances (PICCS)
REACH Reg.	REACH registered substances
TCSI	Taiwan Chemical Substance Inventory
TSCA	Toxic Substance Control Act

## 15.2 Chemical Safety Assessment

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

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## 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 navigation intérieures (European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways)
ADR	Accord européen relatif au transport international des marchandises dangereuses par route (European Agreement concerning the International Carriage of Dangerous Goods by Road)
BCF	Bioconcentration factor
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
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
GHS	"Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Nations
IATA	International Air Transport Association
IATA/DGR	Dangerous Goods Regulations (DGR) for the air transport (IATA)
ICAO	International Civil Aviation Organization
IMDG	International Maritime Dangerous Goods Code
LD50	Lethal Dose 50 %: the LD50 corresponds to the dose of a tested substance causing 50 % lethality during a specified time interval
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
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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**Disclaimer**

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