

Safety data sheet

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BASF Safety data sheet according to UN GHS 4th rev.

Date / Revised: 15.08.2022

Version: 3.0

Product: **beta-Ionone R**

(ID no. 30035178/SDS_GEN_00/EN)

Date of print 12.10.2025

1. Identification

Product identifier

beta-Ionone R

Chemical name: (E)-4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one

CAS Number: 79-77-6

Relevant identified uses of the substance or mixture and uses advised against

Relevant identified uses: Chemical, Chemical for detergents, Cosmetic and oral care chemical, flavoring substance

Details of the supplier of the safety data sheet

Company:

BASF SE

67056 Ludwigshafen

GERMANY

Operating Division Nutrition and Health

Telephone: +49 621 60-48434

E-mail address: EN-global-safety-data@basf.com

Emergency telephone number

International emergency number:

Telephone: +49 180 2273-112

2. Hazards Identification

Classification of the substance or mixture

According to UN GHS criteria

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Aquatic Acute 2
Aquatic Chronic 2

For the classifications not written out in full in this section the full text can be found in section 16.

Label elements

Globally Harmonized System (GHS)

Pictogram:



Hazard Statement:

H401 Toxic to aquatic life.

H411 Toxic to aquatic life with long lasting effects.

Precautionary Statements (Prevention):

P273 Avoid release to the environment.

Precautionary Statements (Response):

P391 Collect spillage.

Precautionary Statements (Disposal):

P501 Dispose of contents and container to hazardous or special waste collection point.

Other hazards

According to UN GHS criteria

If applicable information is provided in this section on other hazards which do not result in classification but which may contribute to the overall hazards of the substance or mixture.

3. Composition/Information on Ingredients

Substances

Chemical nature

(E)-4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one

CAS Number: 79-77-6

EC-Number: 201-224-3

Hazardous ingredients (GHS)

According to UN GHS criteria

(E)-4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one

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Content (W/W): $\geq 75\%$ - $\leq 100\%$	Aquatic Acute 2 Aquatic Chronic 2 H401, H411
CAS Number: 79-77-6	
EC-Number: 201-224-3	
6,10-Dimethylundeca-3,5,9-trien-2-one	
Content (W/W): $> 0\%$ - $< 0,1\%$	Skin Corr./Irrit. 2 Eye Dam./Irrit. 2B Skin Sens. 1B Aquatic Acute 2 Aquatic Chronic 2 H320, H315, H317, H401, H411
CAS Number: 141-10-6	
EC-Number: 205-457-1	

For the classifications not written out in full in this section the full text can be found in section 16.

Mixtures

Not applicable

4. First-Aid Measures

Description of first aid measures

Remove contaminated clothing.

If inhaled:

Keep patient calm, remove to fresh air.

On skin contact:

Wash thoroughly with soap and water

On contact with eyes:

Wash affected eyes for at least 15 minutes under running water with eyelids held open.

On ingestion:

Rinse mouth and then drink 200-300 ml of water.

Most important symptoms and effects, both acute and delayed

Symptoms: Information, i.e. additional information on symptoms and effects may be included in the GHS labeling phrases available in Section 2 and in the Toxicological assessments available in Section 11.

Indication of any immediate medical attention and special treatment needed

Treatment: Symptomatic treatment (decontamination, vital functions).

5. Fire-Fighting Measures

Extinguishing media

Suitable extinguishing media:

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dry powder, carbon dioxide, foam, water spray

Unsuitable extinguishing media for safety reasons:
water jet

Special hazards arising from the substance or mixture

carbon oxides, harmful vapours

The substances/groups of substances mentioned can be released in case of fire.

Advice for fire-fighters

Special protective equipment:

Wear a self-contained breathing apparatus.

Further information:

Dispose of fire debris and contaminated extinguishing water in accordance with official regulations.

Cool endangered containers with water-spray.

6. Accidental Release Measures**Personal precautions, protective equipment and emergency procedures**

Use personal protective clothing. Information regarding personal protective measures, see section 8.

Environmental precautions

Do not discharge into drains/surface waters/groundwater. Inform authorities in the event of product spillage to water courses or sewage systems.

Methods and material for containment and cleaning up

For small amounts: Contain with absorbent material (e.g. sand, silica gel, acid binder, general purpose binder, sawdust).

For large amounts: Dike spillage. Pump off product.

Dispose of absorbed material in accordance with regulations.

7. Handling and Storage**Precautions for safe handling**

Handle in accordance with good industrial hygiene and safety practice.

Protection against fire and explosion:

Take precautionary measures against static discharges. Avoid all sources of ignition: heat, sparks, open flame.

Conditions for safe storage, including any incompatibilities

Odour-sensitive: Segregate from products releasing odours.

Further information on storage conditions: Keep container tightly closed in a cool, well-ventilated place.

Specific end use(s)

For the relevant identified use(s) listed in Section 1 the advice mentioned in this section 7 is to be observed.

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8. Exposure Controls/Personal Protection

Control parameters

Components with occupational exposure limits

No substance specific occupational exposure limits known.

Exposure controls

Personal protective equipment

Respiratory protection:

Respiratory protection in case of vapour/aerosol release. Particle filter with medium efficiency for solid and liquid particles (e.g. EN 143 or 149, Type P2 or FFP2)

Hand protection:

Chemical resistant protective gloves (EN ISO 374-1)

Manufacturer's directions for use should be observed because of great diversity of types.

Eye protection:

Safety glasses with side-shields (frame goggles) (e.g. EN 166)

Body protection:

Body protection must be chosen based on level of activity and exposure.

General safety and hygiene measures

Handle in accordance with good industrial hygiene and safety practice. Wearing of closed work clothing is recommended. No eating, drinking, smoking or tobacco use at the place of work. Hands and/or face should be washed before breaks and at the end of the shift. Store work clothing separately.

9. Physical and Chemical Properties

Information on basic physical and chemical properties

Form:	liquid	
Colour:	colourless to slightly yellow	
Odour:	flowery	
Odour threshold:	< 100 ppm	
pH value:	not applicable	
Melting point:	-35 °C (1.013 hPa) Literature data.	
Boiling point:	267,1 °C (1.013 hPa)	
Flash point:	126 °C	(ISO 2719, closed cup)
Evaporation rate:	Value can be approximated from Henry's Law Constant or vapor pressure.	
Flammability:	hardly combustible	(derived from flash point)

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Lower explosion limit:	For liquids not relevant for classification and labelling., The lower explosion point may be 5 - 15 °C below the flash point.	
Upper explosion limit:	For liquids not relevant for classification and labelling.	
Ignition temperature:	273 °C	(DIN EN 14522)
Vapour pressure:	approx. 0,072 hPa (25 °C) Literature data.	(measured)
Density:	0,9447 g/cm ³ (20 °C) Literature data.	
Relative density:	0,9447 (20 °C) Literature data.	
Relative vapour density (air):	> 1 (20 °C) Heavier than air.	(calculated)
Solubility in water:	0,11 g/l (20 °C)	(OECD Guideline 105)
Solubility (qualitative) solvent(s):	organic solvents readily soluble	
Partitioning coefficient n-octanol/water (log Kow):	4 (25 °C) Literature data.	(OECD Guideline 117)
Self ignition:	Based on its structural properties the product is not classified as self-igniting.	Test type: Spontaneous self-ignition at room-temperature.
Thermal decomposition:	approx. 280 °C (DSC (DIN 51007)) self-accelerating reaction	
Viscosity, dynamic:	11,2 mPa.s (20 °C) 5,04 mPa.s (40 °C)	(OECD 114) (OECD 114)
Viscosity, kinematic:	11,8 mm ² /s (20 °C) 5,43 mm ² /s (40 °C)	(OECD 114) (OECD 114)
Explosion hazard:	Based on the chemical structure there is no indication of explosive properties.	(other)
Fire promoting properties:	not fire-propagating	

Other information

Self heating ability: It is not a substance capable of spontaneous heating.

pKA: The substance does not dissociate.

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Adsorption/water - soil:	KOC: 625,1; log KOC: 2,8	(calculated)
Surface tension:	Based on chemical structure, surface activity is not to be expected.	
Grain size distribution:	The substance / product is marketed or used in a non solid or granular form.	
Molar mass:	192,30 g/mol	

10. Stability and Reactivity

Reactivity

No hazardous reactions if stored and handled as prescribed/indicated.

Corrosion to metals: No corrosive effect on metal.

Formation of flammable gases:	Remarks:	Forms no flammable gases in the presence of water.
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Chemical stability

The product is stable if stored and handled as prescribed/indicated.

Possibility of hazardous reactions

No hazardous reactions if stored and handled as prescribed/indicated.

Conditions to avoid

See SDS section 7 - Handling and storage.

Incompatible materials

Substances to avoid:

None known during use and storage if used according to instructions.

Hazardous decomposition products

Hazardous decomposition products:

No hazardous decomposition products if stored and handled as prescribed/indicated.

11. Toxicological Information

Information on toxicological effects

Acute toxicity

Assessment of acute toxicity:

Virtually nontoxic after a single ingestion. Virtually nontoxic after a single skin contact.

Experimental/calculated data:

LD50 rat (oral): > 4.000 mg/kg

LD50 rat (dermal): > 2.000 mg/kg (OECD Guideline 402)

The product has not been tested. The statement has been derived from substances/products of a similar structure or composition.

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Irritation

Assessment of irritating effects:
Not irritating to the skin. Not irritating to the eyes.

Experimental/calculated data:
Skin corrosion/irritation rabbit: non-irritant (OECD Guideline 404)

Serious eye damage/irritation rabbit: non-irritant (OECD Guideline 405)

Respiratory/Skin sensitization

Assessment of sensitization:
The substance did not cause skin sensitization in humans.

Experimental/calculated data:
guinea pig: Non-sensitizing. (similar to OECD guideline 406)
The product has not been tested. The statement has been derived from substances/products of a similar structure or composition.

human: Non-sensitizing. (Human patch test)
The product has not been tested. The statement has been derived from substances/products of a similar structure or composition.

Germ cell mutagenicity

Assessment of mutagenicity:
Most of the results from the available studies show no evidence of a mutagenic effect. The product has not been fully tested. The statements have been derived in parts from products of a similar structure or composition.

Carcinogenicity

Assessment of carcinogenicity:
The whole of the information assessable provides no indication of a carcinogenic effect.

Reproductive toxicity

Assessment of reproduction toxicity:
The results of animal studies gave no indication of a fertility impairing effect.

Developmental toxicity

Assessment of teratogenicity:
No indications of a developmental toxic / teratogenic effect were seen in animal studies.

Specific target organ toxicity (single exposure)

Assessment of STOT single:
Based on available data, the classification criteria are not met.

Repeated dose toxicity and Specific target organ toxicity (repeated exposure)

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Assessment of repeated dose toxicity:

No substance-specific organotoxicity was observed after repeated administration to animals.

Aspiration hazard

not applicable

12. Ecological Information

Toxicity

Assessment of aquatic toxicity:

Acutely toxic for aquatic organisms. The inhibition of the degradation activity of activated sludge is not anticipated when introduced to biological treatment plants in appropriate low concentrations.

Toxicity to fish:

LC50 (96 h) 5,09 mg/l, Pimephales promelas (EPA 72-1, Flow through.)

The details of the toxic effect relate to the nominal concentration. The product has low solubility in the test medium. An aqueous solution prepared with solubilizers has been tested.

Aquatic invertebrates:

EC50 (48 h) 4,03 mg/l, Daphnia magna (OECD Guideline 202, part 1, static)

The details of the toxic effect relate to the nominal concentration.

Aquatic plants:

EC50 (72 h) 22,15 mg/l (growth rate), Scenedesmus subspicatus (DIN 38412 Part 9, static)

The details of the toxic effect relate to the nominal concentration. The product has low solubility in the test medium. An aqueous solution prepared with solubilizers has been tested.

Microorganisms/Effect on activated sludge:

EC50 (30 min) approx. 1.000 mg/l, activated sludge, domestic (DIN EN ISO 8192-OECD 209-88/302/EEC, P. C, aerobic)

Chronic toxicity to fish:

Study scientifically not justified.

Chronic toxicity to aquatic invertebrates:

Study scientifically not justified.

Assessment of terrestrial toxicity:

No data available concerning terrestrial toxicity.

Study scientifically not justified.

Soil living organisms:

No data available.

Terrestrial plants:

No data available.

Other terrestrial non-mammals:

LD50 > 562 mg/kg, Agelaius phoeniceus

Unspecified

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Persistence and degradability

Assessment biodegradation and elimination (H₂O):
Readily biodegradable (according to OECD criteria).

Elimination information:

70 - 80 % BOD of the ThOD (28 d) (OECD Guideline 301 F) (aerobic, activated sludge, domestic)

Assessment of stability in water:

Substance is readily biodegradable, therefore hydrolysis is not expected to be relevant.

Bioaccumulative potential

Assessment bioaccumulation potential:

Because of the n-octanol/water distribution coefficient (log Pow) accumulation in organisms is possible.

Mobility in soil

Assessment transport between environmental compartments:

Volatility: The substance will slowly evaporate into the atmosphere from the water surface.

Adsorption in soil: Adsorption to solid soil phase is not expected.

Results of PBT and vPvB assessment

According to Annex XIII of Regulation (EC) No.1907/2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH): The product does not fulfill the criteria for PBT (Persistent/bioaccumulative/toxic) and vPvB (very persistent/very bioaccumulative). Self classification

Other adverse effects

The substance is not listed in Regulation (EC) 1005/2009 on substances that deplete the ozone layer.

13. Disposal Considerations

Waste treatment methods

Observe national and local legal requirements.

14. Transport Information

Land transport

ADR

UN number or ID number: UN3082

UN proper shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (BETA-IONONE)

Transport hazard class(es): 9, EHSM

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Packing group: III
Environmental hazards: yes
Special precautions for user: None known

RID

UN number or ID number: UN3082
UN proper shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (BETA-IONONE)

Transport hazard class(es): 9, EHSM
Packing group: III
Environmental hazards: yes
Special precautions for user: None known

Inland waterway transport**ADN**

UN number or ID number: UN3082
UN proper shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (BETA-IONONE)

Transport hazard class(es): 9, EHSM
Packing group: III
Environmental hazards: yes
Special precautions for user: None known

Transport in inland waterway vessel

Not evaluated

Sea transport**IMDG**

UN number or ID number: UN 3082
UN proper shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (BETA-IONONE)

Transport hazard class(es): 9, EHSM
Packing group: III
Environmental hazards: yes
Marine pollutant: YES
Special precautions for user: EmS: F-A; S-F

Air transport

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IATA/ICAO

UN number or ID number: UN 3082

UN proper shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID,
N.O.S. (BETA-IONONE)

Transport hazard class(es): 9, EHSM

Packing group: III

Environmental hazards: yes

Special precautions for user: None known

Maritime transport in bulk according to IMO instruments

Maritime transport in bulk is not intended.

Further information

Product may be shipped as non-hazardous in suitable packages containing a net quantity of 5 L or less under the provisions of various regulatory agencies: ADR, RID, ADN: Special Provision 375; IMDG: 2.10.2.7; IATA: A197; TDG: Special Provision 99(2); 49CFR: §171.4 (c) (2) and also the Special Provision 375 in Appendix B which is regulated in China "Regulations Concerning Road Transportation of Dangerous Goods Part 3: Index of dangerous goods name and transportation requirements" (JT/T 617.3)

15. Regulatory Information**Safety, health and environmental regulations/legislation specific for the substance or mixture**

If other regulatory information applies that is not already provided elsewhere in this safety data sheet, then it is described in this subsection.

16. Other Information

Any other intended applications should be discussed with the manufacturer. Corresponding occupational protection measurements must be followed.

Full text of classifications, hazard symbols and hazard statements, if mentioned in section 2 or 3:

Aquatic Acute	Hazardous to the aquatic environment - acute
Aquatic Chronic	Hazardous to the aquatic environment - chronic
Skin Corr./Irrit.	Skin corrosion/irritation
Eye Dam./Irrit.	Serious eye damage/eye irritation
Skin Sens.	Skin sensitization
H401	Toxic to aquatic life.
H411	Toxic to aquatic life with long lasting effects.
H320	Causes eye irritation.
H315	Causes skin irritation.
H317	May cause an allergic skin reaction.

The data contained in this safety data sheet are based on our current knowledge and experience and describe the product only with regard to safety requirements. This safety data sheet is neither a

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Certificate of Analysis (CoA) nor technical data sheet and shall not be mistaken for a specification agreement. Identified uses in this safety data sheet do neither represent an agreement on the corresponding contractual quality of the substance/mixture nor a contractually designated use. It is the responsibility of the recipient of the product to ensure any proprietary rights and existing laws and legislation are observed.

Vertical lines in the left hand margin indicate an amendment from the previous version.