

Safety data sheet

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BASF Safety data sheet according to Regulation (EC) No. 1907/2006 as amended from time to time.

Date / Revised: 28.01.2016

Version: 5.0

Product: **beta-Ionone R**

(ID no. 30035178/SDS_GEN_EU/EN)

Date of print 02.08.2016

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

1.1. 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

REACH registration number: 01-2119449921-34-0000

1.2. 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

Recommended use: Chemical, flavoring substance, Chemical for detergents, Cosmetic and oral care chemical

For the detailed identified uses of the product see appendix of the safety data sheet.

1.3. 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

1.4. Emergency telephone number

International emergency number:

Telephone: +49 180 2273-112

SECTION 2: Hazards Identification

2.1. Classification of the substance or mixture

According to Regulation (EC) No 1272/2008 [CLP]

Aquatic Chronic 2

H411

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

2.2. Label elements

Globally Harmonized System, EU (GHS)

Pictogram:



Hazard Statement:

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/container to hazardous or special waste collection point.

2.3. Other hazards

According to Regulation (EC) No 1272/2008 [CLP]

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.

SECTION 3: Composition/Information on Ingredients

3.1. 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

For the classifications not written out in full in this section, including the hazard classes and the hazard statements, the full text is listed in section 16.

3.2. Mixtures

Not applicable

SECTION 4: First-Aid Measures

4.1. 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 plenty of water.

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

Symptoms: No significant symptoms are expected due to the non-classification of the product.

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

Treatment: Symptomatic treatment (decontamination, vital functions).

SECTION 5: Fire-Fighting Measures

5.1. Extinguishing media

Suitable extinguishing media:

dry powder, carbon dioxide, foam

5.2. Special hazards arising from the substance or mixture

Burning produces harmful and toxic fumes.

5.3. 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.

SECTION 6: Accidental Release Measures

6.1. Personal precautions, protective equipment and emergency procedures

Ensure adequate ventilation.

6.2. Environmental precautions

Do not discharge into drains/surface waters/groundwater.

6.3. Methods and material for containment and cleaning up

For small amounts: Pick up with absorbent material (e.g. sand, sawdust, general-purpose binder).

For large amounts: Dike spillage. Vacuum up spilled product.

For residues: Pick up with absorbent material (e.g. sand, sawdust, general-purpose binder).

Dispose of absorbed material in accordance with regulations.

6.4. Reference to other sections

Information regarding exposure controls/personal protection and disposal considerations can be found in section 8 and 13.

SECTION 7: Handling and Storage

7.1. Precautions for safe handling

Protection against fire and explosion:

The relevant fire protection measures should be noted.

7.2. Conditions for safe storage, including any incompatibilities

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

Storage stability:

Storage temperature: ≤ 20 °C

7.3. 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.

SECTION 8: Exposure Controls/Personal Protection

8.1. Control parameters

Components with occupational exposure limits

| No occupational exposure limits known.

PNEC

freshwater: 0.07 mg/l

marine water: 0.007 mg/l

intermittent release: 0.7 mg/l

STP: 9 mg/l

sediment (freshwater): 0.0616 mg/kg

sediment (marine water): 0.00616 mg/kg

soil: 0.0156 mg/kg

DNEL

consumer:

Long-term exposure- systemic effects, Inhalation: 3.1 mg/m³

worker:

Long-term exposure- systemic effects, Inhalation: 12.7 mg/m³

consumer:

Long-term exposure- systemic effects, dermal: 3.60 mg/kg

worker:

Long-term exposure- systemic effects, dermal: 6 mg/kg

consumer:

Long-term exposure- systemic effects, oral: 1.80 mg/kg

8.2. Exposure controls

Personal protective equipment

Respiratory protection:

Breathing protection if gases/vapours are formed. Particle filter with medium efficiency for solid and liquid particles (e.g. EN 143 or 149, Type P2 or FFP2)

Hand protection:

Suitable chemical resistant safety gloves (EN 374) also with prolonged, direct contact (Recommended: Protective index 6, corresponding > 480 minutes of permeation time according to EN 374): E.g. nitrile rubber (0.4 mm), chloroprene rubber (0.5 mm), butyl rubber (0.7 mm) etc. Supplementary note: The specifications are based on tests, literature data and information of glove manufacturers or are derived from similar substances by analogy. Due to many conditions (e.g. temperature) it must be considered, that the practical usage of a chemical-protective glove in practice may be much shorter than the permeation time determined through testing.

Eye protection:

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

Body protection:

Body protection must be chosen depending on activity and possible exposure, e.g. apron, protecting boots, chemical-protection suit (according to EN 14605 in case of splashes or EN ISO 13982 in case of dust).

General safety and hygiene measures

Handle in accordance with good industrial hygiene and safety practice. Hands and/or face should be washed before breaks and at the end of the shift.

SECTION 9: Physical and Chemical Properties

9.1. 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	(DIN EN 22719; ISO 2719, closed cup)
Evaporation rate:	not determined	
Flammability:	not flammable	
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)

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Vapour pressure:	approx. 0.072 hPa (25 °C)	(measured)
Density:	Literature data. 0.9447 g/cm ³ (20 °C)	
Relative density:	Literature data. 0.9447 (20 °C)	
Relative vapour density (air):	Literature data. not determined	
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)	(OECD Guideline 117)
Self ignition:	Literature data. Based on its structural properties the product is not classified as self-igniting.	Test type: Spontaneous self-ignition at room-temperature.
Thermal decomposition:	not determined	
Viscosity, dynamic:	11.2 mPa.s (20 °C)	(OECD 114)
	5.04 mPa.s (40 °C)	(OECD 114)
Viscosity, kinematic:	11.8 mm ² /s (20 °C)	(OECD 114)
	5.43 mm ² /s (40 °C)	(OECD 114)
Explosion hazard:	Based on the chemical structure there is no indicating of explosive properties.	(other)
Fire promoting properties:	not fire-propagating	

9.2. Other information

Self heating ability:	It is not a substance capable of spontaneous heating.
pKA:	The substance does not dissociate.
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

SECTION 10: Stability and Reactivity

10.1. Reactivity

Corrosion to metals:	No corrosive effect on metal.	
Formation of flammable gases:	Remarks:	Forms no flammable gases in the presence of water.

10.2. Chemical stability

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

10.3. Possibility of hazardous reactions

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

10.4. Conditions to avoid

Avoid all sources of ignition: heat, sparks, open flame.

10.5. Incompatible materials

Substances to avoid:
No substances known that should be avoided.

10.6. Hazardous decomposition products

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

SECTION 11: Toxicological Information

11.1. 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.

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)

Assessment of repeated dose toxicity:

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

Aspiration hazard

not applicable

SECTION 12: Ecological Information

12.1. 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:

Study scientifically not justified.

12.2. 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:

Study scientifically not justified.

12.3. Bioaccumulative potential

Bioaccumulation potential:

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

12.4. 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 expected.

12.5. 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

12.6. Other adverse effects

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

SECTION 13: Disposal Considerations

13.1. Waste treatment methods

Observe national and local legal requirements.

SECTION 14: Transport Information

Land transport

ADR

UN number	UN3082
UN proper shipping name:	ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (contains BETA-IONONE)
Transport hazard class(es):	9, EHSM
Packing group:	III
Environmental hazards:	yes
Special precautions for user:	Tunnel code: E

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RID

UN number: UN3082
UN proper shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID,
N.O.S. (contains 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: UN3082
UN proper shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID,
N.O.S. (contains 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: UN 3082
UN proper shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID,
N.O.S. (contains BETA-IONONE)
Transport hazard class(es): 9, EHSM
Packing group: III
Environmental hazards: yes
Marine pollutant: YES
Special precautions for user: None known

Air transport**IATA/ICAO**

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

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

14.1. UN number

See corresponding entries for "UN number" for the respective regulations in the tables above.

14.2. UN proper shipping name

See corresponding entries for "UN proper shipping name" for the respective regulations in the tables above.

14.3. Transport hazard class(es)

See corresponding entries for "Transport hazard class(es)" for the respective regulations in the tables above.

14.4. Packing group

See corresponding entries for "Packing group" for the respective regulations in the tables above.

14.5. Environmental hazards

See corresponding entries for "Environmental hazards" for the respective regulations in the tables above.

14.6. Special precautions for user

See corresponding entries for "Special precautions for user" for the respective regulations in the tables above.

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

Regulation: Not evaluated
Shipment approved: Not evaluated
Pollution name: Not evaluated
Pollution category: Not evaluated
Ship Type: Not evaluated

SECTION 15: Regulatory Information

15.1. 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.

SECTION 16: Other Information

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Assessment of the hazard classes according to UN GHS criteria (most recent version)

Aquatic Acute 2

Aquatic Chronic 2

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

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

Aquatic Chronic

Hazardous to the aquatic environment - chronic

|H411

Toxic to aquatic life with long lasting effects.

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. The data do not describe the product's properties (product specification). Neither should any agreed property nor the suitability of the product for any specific purpose be deduced from the data contained in the safety data sheet. 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.