

Safety data sheet

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BASF Safety data sheet
Date / Revised: 27.01.2025
Product: **Citronellylnitrile**

Version: 10.1

(30035072/SDS_GEN_SG/EN)

Date of print: 08.10.2025

1. Substance/preparation and manufacturer/supplier identification

Product name:
Citronellylnitrile

Use: Chemical, Chemical for detergents, Chemical for soaps, detergents and cosmetic

Manufacturer/supplier:

BASF South East Asia Pte Ltd.
128 Beach Road #18-01
Guoco Midtown, 189773, Singapore
Telephone: +65 8322 4420
Telefax number: +65 6 334-0330
E-mail address: benny.zou@basf.com

Emergency information:

Singapore Emergency Toll-Free Number:
Telephone: 1800-723-1361
International emergency number:
Telephone: +49 180 2273-112

2. Hazard identification

Classification of the substance and mixture:
Acute toxicity: Cat.5 (oral)
Hazardous to the aquatic environment - acute: Cat.3

Label elements and precautionary statement:

Signal Word:
Warning

Hazard Statement:

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H303 May be harmful if swallowed.
H402 Harmful to aquatic life.

Precautionary Statements (Prevention):

P273 Avoid release to the environment.

Precautionary Statements (Response):

P301 + P312 IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell.

Precautionary Statements (Disposal):

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

Other hazards which do not result in classification:

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

Chemical nature

Substance nature: Substance

3,7-dimethyloct-6-enenitrile
CAS Number: 51566-62-2

Hazardous ingredients

3,7-dimethyloct-6-enenitrile
Content (W/W): $\geq 75\%$ - $\leq 100\%$ Acute Tox.: Cat. 5 (oral)
Aquatic Acute: Cat. 3
CAS Number: 51566-62-2

4. First-Aid Measures

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:

Immediately rinse mouth and then drink 200-300 ml of water, seek medical attention.

Note to physician:

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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.

Treatment: Symptomatic treatment (decontamination, vital functions).

5. Fire-Fighting Measures

Suitable extinguishing media:
carbon dioxide, foam, dry powder, water spray

Unsuitable extinguishing media for safety reasons:
water jet

Specific hazards:
carbon oxides, harmful vapours
The substances/groups of substances mentioned can be released in case of fire.

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

Environmental precautions:
Do not discharge into drains/surface waters/groundwater.

Methods for cleaning up or taking 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

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.

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Storage

Further information on storage conditions: Keep container tightly closed and dry; store in a cool place.

8. Exposure controls and personal protection

Components with occupational exposure limits

No substance specific occupational exposure limits known.

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)

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

Form:	liquid
Colour:	colourless
Odour:	fruity
Odour threshold:	< 100 ppm

pH value:

The substance does not dissociate.

glass transition temperature: -120 °C

(OECD Guideline 102)

Melting point:

(OECD Guideline 102)

Boiling point: not applicable
231.43 °C
(1,013.25 hPa)

(measured)

Flash point: 103 °C

(DIN 51758, closed cup)

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Evaporation rate:	Value can be approximated from Henry's Law Constant or vapor pressure.	
Flammability (solid/gas):	hardly combustible	(derived from flash point)
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:	307 °C	(Directive 92/69/EEC, A.15)
Thermal decomposition:	approx. 380 °C No decomposition if stored and handled as prescribed/indicated.	(DSC (DIN 51007))
Self ignition:	Based on its structural properties the product is not classified as self-igniting.	Test type: Spontaneous self-ignition at room-temperature.
Self heating ability:	It is not a substance capable of spontaneous heating.	
SADT:	No data available.	
Explosion hazard:	not explosive	(other)
Fire promoting properties:	Based on its structural properties the product is not classified as oxidizing.	
Vapour pressure:	0.57 mbar (50 °C) 0.05 mbar (20 °C)	(measured) (measured)
Density:	0.8453 g/cm ³ (20 °C)	(OECD Guideline 109)
Relative density:	0.8453 (20 °C)	(OECD Guideline 109)
Relative vapour density (air):	> 1 (20 °C) Heavier than air.	(calculated)
Solubility in water:	119 g/l (20 °C)	
Solubility (qualitative) solvent(s):	organic solvents soluble	
Partitioning coefficient n-octanol/water (log Pow):	3.55 The data refers to the undissociated form of the substance. 3.1 (23 °C; pH value: 6.2)	(calculated) (OECD Guideline 117)

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Viscosity, dynamic:	2.5 mPa.s (20 °C) The value was determined by calculation from the detected kinematic viscosity. 1.64 mPa.s (40 °C) The value was determined by calculation from the detected kinematic viscosity.	(OECD Guideline 114) (OECD Guideline 114)
Viscosity, kinematic:	2.96 mm ² /s (20 °C) 1.97 mm ² /s (40 °C)	(OECD Guideline 114) (OECD Guideline 114)
Molar mass:	151.25 g/mol	

Particle characteristics

Particle size distribution: The substance / product is marketed or used in a non solid or granular form. -

Specific Surface Area:
No data available.

Particle Shape:
No data available.

Dustiness:
No data available.

10. Stability and Reactivity

Conditions to avoid:
See SDS section 7 - Handling and storage.

Thermal decomposition: approx. 380 °C (DSC (DIN 51007))
No decomposition if stored and handled as
prescribed/indicated.

Substances to avoid:
acids

Corrosion to metals: No corrosive effect on metal.

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

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

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

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

11. Toxicological Information

Routes of exposure

Acute oral toxicity

Experimental/calculated data:
LD50rat (oral): 4,490 mg/kg

Acute inhalation toxicity

LC50 rat (by inhalation): > 4.9 mg/l 4 h (BASF-Test)
An aerosol was tested.

Acute dermal toxicity

LD50 rabbit (dermal): > 5,000 mg/kg

Assessment of acute toxicity

Of low toxicity after single ingestion. Virtually nontoxic after a single skin contact. Virtually nontoxic by inhalation.

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.

Irritation

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

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

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

Respiratory/Skin sensitization

Assessment of sensitization:
Skin sensitizing effects were not observed in animal studies. A controlled medical study in humans did not reveal a skin sensitizing effect.

Experimental/calculated data:
Draize test guinea pig: Non-sensitizing. (other)

Human Maximization Test human: Non-sensitizing. (other)

Germ cell mutagenicity

Assessment of mutagenicity:
In the majority of tests performed (bacteria/microorganisms/cell cultures) a mutagenic effect was not found. A mutagenic effect was also not observed in in-vivo assays.

Carcinogenicity

Assessment of carcinogenicity:

No data available concerning carcinogenic effects.

Experimental/calculated data:

No data available.

Reproductive toxicity

Assessment of reproduction toxicity:

The results of animal studies gave no indication of a fertility impairing effect.

Developmental toxicity

Assessment of teratogenicity:

Animal studies gave no indication of a developmental toxic effect at doses that were not toxic to the parental animals.

Specific target organ toxicity (single exposure)

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

No data available.

12. Ecological Information

Ecotoxicity

Assessment of aquatic toxicity:

Acutely harmful 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) 31.58 mg/l, *Leuciscus idus* (DIN 38412 Part 15, static)

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

Aquatic invertebrates:

EC50 (48 h) 11.4 mg/l, *Daphnia magna* (OECD Guideline 202, part 1, static)

Aquatic plants:

EC50 (72 h) 14.5 mg/l (growth rate), *Pseudokirchneriella subcapitata* (OECD Guideline 201, static)

Microorganisms/Effect on activated sludge:

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EC10 (30 min) > 10,000 mg/l, *Pseudomonas putida* (DIN 38412 Part 27 (draft), aquatic)

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

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.

Soil living organisms:

Study scientifically not justified.

Terrestrial plants:

Study scientifically not justified.

Other terrestrial non-mammals:

Study scientifically not justified.

Mobility

Assessment transport between environmental compartments:

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

Adsorption to solid soil phase is possible.

Persistence and degradability

Elimination information:

69 % BOD of the ThOD (28 d) (OECD 301F; ISO 9408; 92/69/EWG, C.4-D) (aerobic, activated sludge, domestic)

Assessment of stability in water:

Study scientifically not justified.

Bioaccumulation potential

Assessment bioaccumulation potential:

Because of the n-octanol/water distribution coefficient (log Pow) accumulation in organisms is not to be expected.

13. Disposal Considerations

Observe national and local legal requirements.

Contaminated packaging:

Uncontaminated packaging can be re-used.

Packs that cannot be cleaned should be disposed of in the same manner as the contents.

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14. Transport Information

Domestic transport:

	Not classified as a dangerous good under transport regulations
UN number or ID number	Not applicable
UN proper shipping name:	Not applicable
Transport hazard class(es):	Not applicable
Packing group:	Not applicable
Environmental hazards:	Not applicable
Special precautions for user	None known

Sea transport

IMDG

	Not classified as a dangerous good under transport regulations
UN number or ID number:	Not applicable
UN proper shipping name:	Not applicable
Transport hazard class(es):	Not applicable
Packing group:	Not applicable
Environmental hazards:	Not applicable
	Marine pollutant: no
Special precautions for user	None known

Air transport

IATA/ICAO

	Not classified as a dangerous good under transport regulations
UN number or ID number	Not applicable
Proper shipping name:	Not applicable
Transport hazard class(es):	Not applicable
Packing group:	Not applicable
Environmental hazards:	Not applicable
Special precautions for user	None known

Maritime transport in bulk according to IMO instruments

Maritime transport in bulk is not intended.

15. Regulatory Information

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Other regulations

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.

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

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 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.