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Safety data sheet

BASF Safety data sheet according to UN GHS 4th rev.
Date / Revised: 24.08.2022 Version: 3.0
Product: **Citronellylnitrile**

(ID no. 30035072/SDS_GEN_00/EN)
Date of print 11.10.2025

1. Identification

Product identifier

Citronellylnitrile

Chemical name: 3,7-Dimethyloct-6-enenitrile
CAS Number: 51566-62-2

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

Relevant identified uses: Chemical, Chemical for detergents, Chemical for soaps, detergents and cosmetic

Details of the supplier of the safety data sheet

Company:
BASF SE
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GERMANY
Operating Division Nutrition and Health

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International emergency number:
Telephone: +49 180 2273-112

2. Hazards Identification

Classification of the substance or mixture

According to UN GHS criteria

Acute Tox. 5 (oral)
Aquatic Acute 3

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)

Signal Word:
Warning

Hazard Statement:

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

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

3,7-Dimethyloct-6-enenitrile
CAS Number: 51566-62-2
EC-Number: 257-288-8

Hazardous ingredients (GHS)
According to UN GHS criteria

3,7-Dimethyloct-6-enenitrile

Content (W/W): >= 75 % - <= 100 %	Acute Tox. 5 (oral)
	Aquatic Acute 3
CAS Number: 51566-62-2	H303, H402
EC-Number: 257-288-8	

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

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.

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:
carbon dioxide, foam, dry powder, 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.

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

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

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)

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	
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)
	not applicable	
Boiling point:	231,43 °C (1.013,25 hPa)	(measured)
Flash point:	103 °C	(DIN 51758, closed cup)
Evaporation rate:		
	Value can be approximated from Henry's Law Constant or vapor pressure.	
Flammability:	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)
Vapour pressure:	0,57 mbar (50 °C)	(measured)
	0,05 mbar (20 °C)	(measured)
Density:	0,8453 g/cm3 (20 °C)	(OECD Guideline 109)

Relative density:	0,8453 (20 °C)	(OECD Guideline 109)
Relative vapour density (air):> 1		(calculated)
	(20 °C) Heavier than air.	
Solubility in water:		(OECD Guideline 105)
	119 g/l (20 °C)	
Solubility (qualitative) solvent(s):	organic solvents soluble	
Partitioning coefficient n-octanol/water (log Kow):	3,55 The data refers to the undissociated form of the substance.	(calculated)
	3,1 (23 °C; pH value: 6,2)	(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. 380 °C (DSC (DIN 51007)) No decomposition if stored and handled as prescribed/indicated.	
Viscosity, dynamic:	2,5 mPa.s (20 °C) The value was determined by calculation from the detected kinematic viscosity.	(OECD 114)
	1,64 mPa.s (40 °C) The value was determined by calculation from the detected kinematic viscosity.	(OECD 114)
Viscosity, kinematic:	2,96 mm2/s (20 °C)	(OECD 114)
	1,97 mm2/s (40 °C)	(OECD 114)
Explosion hazard:	not explosive	(other)
Fire promoting properties:	Based on its structural properties the product is not classified as oxidizing.	

Other information

Self heating ability:	It is not a substance capable of spontaneous heating.
pKA:	The substance does not dissociate.
Grain size distribution:	The substance / product is marketed or used in a non solid or granular form.
Molar mass:	151,25 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.

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:
acids

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

Experimental/calculated data:
LD50 rat (oral): 4.490 mg/kg

LC50 rat (by inhalation): > 4,9 mg/l 4 h (BASF-Test)
An aerosol was tested.

LD50 rabbit (dermal): > 5.000 mg/kg

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.

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)

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 organtoxicity was observed after repeated administration to animals.

Aspiration hazard

No data available.

12. Ecological Information

Toxicity

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:
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.

Persistence and degradability

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

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

Assessment of stability in water:
Study scientifically not justified.

Bioaccumulative potential

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

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 possible.

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.

Contaminated packaging:
Uncontaminated packaging can be re-used.
Packs that cannot be cleaned should be disposed of in the same manner as the contents.

14. Transport Information

Land transport

ADR

	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

RID

	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

Inland waterway transport

ADN

	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

Transport in inland waterway vessel
Not evaluated

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
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
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

Maritime transport in bulk according to IMO instruments

Maritime transport in bulk is not intended.

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:

Acute Tox.	Acute toxicity
Aquatic Acute	Hazardous to the aquatic environment - acute
H303	May be harmful if swallowed.
H402	Harmful to aquatic life.

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.

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