We create chemistry

Safety data sheet

1. Identification

Product identifier

Tetrahydrolinalool

Chemical name: 3,7-Dimethyloctan-3-ol
CAS Number: 78-69-3

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

Eye Dam./Irrit. 2A
Skin Corr./Irrit. 2
Flam. Liq. 4
Skin Sens. 1B
Aquatic Acute 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:

Signal Word:
Warning

Hazard Statement:

H227	Combustible liquid.
H319	Causes serious eye irritation.
H315	Causes skin irritation.
H317	May cause an allergic skin reaction.
H401	Toxic to aquatic life.

Precautionary Statements (Prevention):

P280	Wear protective gloves and eye protection or face protection.
P261	Avoid breathing mist or vapour or spray.
P280	Wear eye protection.
P273	Avoid release to the environment.
P210	Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P272	Contaminated work clothing should not be allowed out of the workplace.
P264	Wash contaminated body parts thoroughly after handling.

Precautionary Statements (Response):

P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P302 + P352	IF ON SKIN: Wash with plenty of soap and water.
P333 + P313	If skin irritation or rash occurs: Get medical attention.
P332 + P313	If skin irritation occurs: Get medical attention.
P362 + P364	Take off contaminated clothing and wash it before reuse.
P337 + P313	If eye irritation persists: Get medical attention.
P370 + P378	In case of fire: Use extinguishing powder, foam or CO2 for extinction.

Precautionary Statements (Storage):

P403	Store in a well-ventilated place.

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-Dimethyloctan-3-ol
CAS Number: 78-69-3
EC-Number: 201-133-9

Hazardous ingredients (GHS)
According to UN GHS criteria

3,7-Dimethyloctan-3-ol

Content (W/W): >= 75 % - <= 100 %	Flam. Liq. 4
CAS Number: 78-69-3	Skin Corr./Irrit. 2
EC-Number: 201-133-9	Eye Dam./Irrit. 2A
	Skin Sens. 1B
	Aquatic Acute 2
	H227, H319, H315, H317, H401

Linalool

Content (W/W): > 0 % - < 0,1 %	Flam. Liq. 4
CAS Number: 78-70-6	Acute Tox. 5 (oral)
EC-Number: 201-134-4	Skin Corr./Irrit. 2
	Eye Dam./Irrit. 2A
	Skin Sens. 1B
	Aquatic Acute 3
	H227, H319, H315, H303, H317, H402

Geraniol

Content (W/W): > 0 % - < 0,1 %	Acute Tox. 5 (oral)
CAS Number: 106-24-1	Skin Corr./Irrit. 2
EC-Number: 203-377-1	Eye Dam./Irrit. 1
	Skin Sens. 1
	Aquatic Acute 3
	H318, H315, H303, H317, H402

Citral

Content (W/W): > 0 % - < 0,1 %	Acute Tox. 5 (oral)
CAS Number: 5392-40-5	Acute Tox. 5 (dermal)
EC-Number: 226-394-6	Skin Corr./Irrit. 2
INDEX-Number: 605-019-00-3	Eye Dam./Irrit. 2A
	Skin Sens. 1
	Aquatic Acute 2
	H319, H315, H317, H303 + H313, H401

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, seek medical attention.

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, consult an eye specialist.

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: Treat according to symptoms (decontamination, vital functions), no known specific antidote.

5. Fire-Fighting Measures

Extinguishing media

Suitable extinguishing media:
carbon dioxide, dry powder, foam

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. Combustible Liquid

Advice for fire-fighters
Special protective equipment:
Wear self-contained breathing apparatus and chemical-protective clothing.

Further information:
Collect contaminated extinguishing water separately, do not allow to reach sewage or effluent systems. 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. Ensure adequate ventilation. Do not breathe vapour/spray. Avoid contact with the skin, eyes and clothing.

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

Methods and material for containment and cleaning up
For large amounts: Dike spillage. Cover with blanket of foam (alcohol-resistant foam). Pump off product.
For residues: Contain with absorbent material (e.g. sand, silica gel, acid binder, general purpose binder, sawdust).
Dispose of absorbed material in accordance with regulations.

7. Handling and Storage

Precautions for safe handling
Ensure thorough ventilation of stores and work areas. Wear suitable protective clothing and eye/face protection. Avoid contact with the skin, eyes and clothing. Keep container tightly sealed. This product may cause irritations; wash your hands after every contact.

Protection against fire and explosion:
The product is combustible. Avoid all sources of ignition: heat, sparks, open flame. Take precautionary measures against static discharges. If exposed to fire, keep containers cool by spraying with water. Vapours may form explosive mixture with air.

Conditions for safe storage, including any incompatibilities
Odour-sensitive: Segregate from products releasing odours.
Further information on storage conditions: Keep container tightly closed and dry; store in a cool place. Protect containers from physical damage. Protect from direct sunlight.

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:
Suitable respiratory protection for higher concentrations or long-term effect: Gas filter for gases/vapours of organic compounds (boiling point >65 °C, e. g. EN 14387 Type A)

Hand protection:
Suitable chemical resistant safety gloves (EN ISO 374-1) also with prolonged, direct contact (Recommended: Protective index 6, corresponding > 480 minutes of permeation time according to EN ISO 374-1): 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. 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 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. Avoid contact with the skin, eyes and clothing. 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:	flowery, sweetish
Odour threshold:	< 100 ppm
pH value:	7
Freezing point:	-56 °C (1.013 hPa) Literature data.

Boiling point:	197 °C (1.013,25 hPa)	(measured)
Flash point:	77 °C	(DIN 51758, closed cup)
Evaporation rate:	Value can be approximated from Henry's Law Constant or vapor pressure.	
Flammability:	Combustible liquid.	(derived from flash point)
Lower explosion limit:	1,3 %(V) (74 °C)	(air)
Upper explosion limit:	For liquids not relevant for classification and labelling.	
Ignition temperature:	360 °C	(DIN 51794)
Vapour pressure:	1 mbar (20 °C) 3 mbar (50 °C)	
Density:	0,826 g/cm3 (25 °C) Literature data.	
Relative density:	0,826 (25 °C)	
Relative vapour density (air):	> 1 (20 °C) Heavier than air.	(calculated)
Solubility in water:	0,320 g/l (25 °C, 1.013 hPa)	
Solubility (qualitative) solvent(s):	organic solvents soluble	
Partitioning coefficient n-octanol/water (log Kow):	3,3 (20 - 23 °C)	(OECD Guideline 107)
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. 470 °C (DSC (DIN 51007))	
Viscosity, dynamic:	11,063 mPa.s (25 °C) Literature data.	
Viscosity, kinematic:	17,4 mm2/s (23 °C)	
Explosion hazard:	Based on the chemical structure there is no indication of explosive properties.	
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.

Adsorption/water - soil:	KOC: 56,3; log KOC: 1,75	(calculated)
Surface tension:	26,78 mN/m (25 °C; 100 %(V))	
Grain size distribution:	The substance / product is marketed or used in a non solid or granular form.	
Molar mass:	158,28 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
Reacts with acids.

Conditions to avoid
Avoid all sources of ignition: heat, sparks, open flame. 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. Inhalation-risk test (IRT): No mortality within 8 hours as shown in animal studies. The inhalation of a highly saturated vapor-air mixture represents no acute hazard.

Experimental/calculated data:
LD50 rat (oral): 8.270 mg/kg (BASF-Test)

rat (by inhalation): 8 h (IRT)

Inhalation-risk test (IRT): No mortality within 8 hours as shown in animal studies. The inhalation of a highly saturated vapor-air mixture represents no acute hazard.

LD50 rabbit (dermal): > 5.000 mg/kg

Irritation

Assessment of irritating effects:
Skin contact causes irritation. Eye contact causes irritation.

Experimental/calculated data:
Skin corrosion/irritation rabbit: Irritant. (BASF-Test)

Skin corrosion/irritation human: Irritant. (OECD Guideline 439)

Serious eye damage/irritation rabbit: Irritant. (BASF-Test)

Respiratory/Skin sensitization

Assessment of sensitization:
Caused skin sensitization in animal studies.

Experimental/calculated data:
Mouse Local Lymph Node Assay (LLNA) mouse: skin sensitizing (OECD Guideline 429)

Germ cell mutagenicity

Assessment of mutagenicity:
No mutagenic effect was found in various tests with bacteria and mammalian cell culture.

Carcinogenicity

Assessment of carcinogenicity:
Study does not need to be conducted.

Reproductive toxicity

Assessment of reproduction toxicity:
The results of animal studies gave no indication of a fertility impairing effect. The product has not been tested. The statement has been derived from substances/products of a similar structure or composition.

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

Specific target organ toxicity (single exposure)

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

Remarks: 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:
Effects on the kidney of male rats were detected after repeated exposure. These effects are specific for the male rat and are known to be of no relevance to humans. The product has not been tested. The statement has been derived from substances/products of a similar structure or composition.

Aspiration hazard

No data available.

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) 8,9 mg/l, Brachydanio rerio (OECD Guideline 203, semistatic)
Nominal concentration.

Aquatic invertebrates:
EC50 (48 h) 14,2 mg/l, Daphnia magna (OECD Guideline 202, part 1, static)
The statement of the toxic effect relates to the analytically determined concentration.

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

Microorganisms/Effect on activated sludge:
EC10 (0,5 h) 450 mg/l, Pseudomonas putida (DIN 38412 Part 27 (draft), aquatic)
The product has low solubility in the test medium. An aqueous solution prepared with solubilizers has been tested.

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.

Persistence and degradability

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

Elimination information:

approx. 60 - 70 % BOD of the ThOD (28 d) (OECD 301F; ISO 9408; 92/69/EEC, C.4-D) (aerobic, activated sludge, domestic) Readily biodegradable (according to OECD criteria).

Assessment of stability in water:
Substance is readily biodegradable, therefore hydrolysis is not expected to be relevant.

Bioaccumulative potential

Assessment bioaccumulation potential:
Significant accumulation in organisms is not to be expected.
The product has not been tested. The statement has been derived from the structure of the product.

Bioaccumulation potential:
Bioconcentration factor: 99,87 (calculated)
The product has not been tested. The statement has been derived from the structure of the product.

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

	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	None known

user

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:

Eye Dam./Irrit.	Serious eye damage/eye irritation
Skin Corr./Irrit.	Skin corrosion/irritation
Flam. Liq.	Flammable liquids
Skin Sens.	Skin sensitization
Aquatic Acute	Hazardous to the aquatic environment - acute
Acute Tox.	Acute toxicity
H227	Combustible liquid.
H319	Causes serious eye irritation.
H315	Causes skin irritation.
H317	May cause an allergic skin reaction.
H401	Toxic to aquatic life.
H303	May be harmful if swallowed.
H402	Harmful to aquatic life.
H318	Causes serious eye damage.
H303 + H313	May be harmful if swallowed or in contact with skin

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.