

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: 19.04.2016

Version: 4.0

Product: **Tetrahydroinalool**

(ID no. 30034995/SDS_GEN_EU/EN)

Date of print 20.04.2016

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

1.1. Product identifier

Tetrahydroinalool

Chemical name: 3,7-Dimethyloctan-3-ol

CAS Number: 78-69-3

REACH registration number: 01-2119454788-21-0000

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

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]

Skin Corr./Irrit. 2

Eye Dam./Irrit. 2

| H319, H315

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

2.2. Label elements

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

Pictogram:



Signal Word:

Warning

Hazard Statement:

H319 Causes serious eye irritation.

H315 Causes skin irritation.

Precautionary Statements (Prevention):

| P280 Wear protective gloves and eye/face protection.

P264 Wash with plenty of water and soap 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.

| P303 + P352 IF ON SKIN (or hair): Wash with plenty of soap and water.

P332 + P313 If skin irritation occurs: Get medical advice/attention.

P337 + P311 If eye irritation persists: Call a POISON CENTER or doctor/physician.

| P362 + P364 Take off contaminated clothing and wash it before reuse.

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. The

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product does not contain a substance fulfilling the PBT (persistent/bioaccumulative/toxic) criteria or the vPvB (very persistent/very bioaccumulative) criteria.

SECTION 3: Composition/Information on Ingredients

3.1. Substances

Chemical nature

3,7-Dimethyloctan-3-ol

CAS Number: 78-69-3

EC-Number: 201-133-9

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, 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.

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

Symptoms: The most important known symptoms and effects are described in the labelling (see section 2) and/or in section 11.

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

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

SECTION 5: Fire-Fighting Measures

5.1. Extinguishing media

Suitable extinguishing media:
carbon dioxide, dry powder

Unsuitable extinguishing media for safety reasons:
water

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 self-contained breathing apparatus and chemical-protective clothing.

Further information:

Keep containers cool by spraying with water if exposed to fire. Collect contaminated extinguishing water separately, do not allow to reach sewage or effluent systems. Fire debris must be disposed of 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 large amounts: Dike spillage. Pump off product.

For residues: Pick up with suitable absorbent material. 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

Ensure thorough ventilation of stores and work areas.

Protection against fire and explosion:

Prevent electrostatic charge - sources of ignition should be kept well clear - fire extinguishers should be kept handy.

7.2. Conditions for safe storage, including any incompatibilities

Suitable materials for containers: Aluminium, High density polyethylene (HDPE), tinned carbon steel (Tinplate), glass, Low density polyethylene (LDPE), Stove-lacquer RDL 50, Stainless steel 1.4301 (V2), Stainless steel 1.4401

Further information on storage conditions: Protect from air. Protect contents from the effects of light. Containers should be stored tightly sealed in a dry place. Protect against heat.

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

none

| No occupational exposure limits known.

PNEC

freshwater: 0.0089 mg/l

marine water: 0.00089 mg/l

intermittent release: 0.089 mg/l

STP: 450 mg/l

sediment (freshwater): 0.0821 mg/kg

sediment (marine water): 0.00821 mg/kg

soil: 0.0112 mg/kg

oral (secondary poisoning): 0.0023 mg/kg

DNEL

worker:

Long-term exposure- systemic effects, Inhalation: 2.75 mg/m³

worker:

Long-term exposure- systemic effects, dermal: 2.5 mg/kg bw/day

worker:

Short-term exposure - local effects, dermal: 2.76 mg/cm²

consumer:

Long-term exposure- systemic effects, Inhalation: 0.68 mg/m³

consumer:

Long-term exposure- systemic effects, oral: 0.2 mg/kg bw/day

consumer:

Long-term exposure- systemic effects, dermal: 1.25 mg/kg bw/day

consumer:

Short-term exposure - local effects, dermal: 2.76 mg/cm²

8.2. Exposure controls

Personal protective equipment

Respiratory protection:

Wear respiratory protection if ventilation is inadequate. 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 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. Avoid contact with the skin, eyes and clothing. Wearing of closed work clothing is recommended. Keep away from food, drink and animal feeding stuffs. No eating, drinking, smoking or tobacco use at the place of work.

SECTION 9: Physical and Chemical Properties**9.1. 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:	not determined	
Flammability:	not readily ignited	
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:	11.1 Pa (19.6 °C) Literature data.	(measured)
Density:	0.826 g/cm ³ (25 °C) Literature data.	
Relative density:	0.826 (25 °C)	
Relative vapour density (air):	not determined	
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:	> 200 °C	
Viscosity, dynamic:	11.063 mPa.s (25 °C) Literature data.	
Viscosity, kinematic:	17.4 mm ² /s (23 °C)	

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Explosion hazard: Based on the chemical structure there is no indicating of explosive properties.

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.

Adsorption/water - soil: KOC: 56.3; log KOC: 1.75 (calculated)

Volatility/water - air: (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

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

Reacts with acids.

10.4. Conditions to avoid

See MSDS section 7 - Handling and storage.

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. 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)

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:

Skin sensitizing effects were not observed in animal studies. The product has not been tested. The statement has been derived from substances/products of a similar structure or composition.

Experimental/calculated data:

Skin painting test guinea pig: Non-sensitizing.

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:

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.

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.

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) 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:

Study scientifically not justified.

12.2. Persistence and degradability

Assessment biodegradation and elimination (H₂O):

Readily biodegradable (according to OECD criteria).

Elimination information:

approx. 60 - 70 % (28 d) (OECD 301F; ISO 9408; 92/69/EEC, C.4-D) (aerobic, activated sludge, domestic)

12.3. Bioaccumulative potential

Assessment bioaccumulation potential:

Significant accumulation in organisms is not to be expected.

Bioaccumulation potential:

Bioconcentration factor: 99.87 (calculated)

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 not 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.

12.7. Additional information

Other ecotoxicological advice:
Do not release untreated into natural waters.

SECTION 13: Disposal Considerations

13.1. Waste treatment methods

Observe national and local legal requirements.

SECTION 14: Transport Information

Land transport

ADR

	Not classified as a dangerous good under transport regulations
UN 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:	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:	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:	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:	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

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

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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

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

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

Skin Corr./Irrit.	Skin corrosion/irritation
Eye Dam./Irrit.	Serious eye damage/eye irritation
H319	Causes serious eye irritation.
H315	Causes skin irritation.

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

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responsibility of the recipient of the product to ensure any proprietary rights and existing laws and legislation are observed.

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