

Chemical Safety Data Sheet MSDS / SDS

3,7-DIMETHYL-1-OCTANOL

Revision Date:2023-11-29 Revision Number:1

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

Product name : 3,7-DIMETHYL-1-OCTANOL
CBnumber : CB6103633
CAS : 106-21-8
EINECS Number : 203-374-5
Synonyms : TETRAHYDROGERANIOL,Dihydrocitronello

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

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.
Uses advised against : none

Company Identification

Company : Chemicalbook
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone : 400-158-6606

SECTION 2: Hazards identification**GHS Label elements, including precautionary statements**

Symbol(GHS)



Signal word

Warning

Precautionary statements

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.

Continuerinsing.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P264 Wash skin thoroughly after handling.

P264 Wash hands thoroughly after handling.

Hazard statements

H411 Toxic to aquatic life with long lasting effects

H319 Causes serious eye irritation

H315 Causes skin irritation

SECTION 3: Composition/information on ingredients

Substance

Product name	: 3,7-DIMETHYL-1-OCTANOL
Synonyms	: TETRAHYDROGERANIOL, Dihydrocitronellol
CAS	: 106-21-8
EC number	: 203-374-5
MF	: C10H22O
MW	: 158.28

SECTION 4: First aid measures

Description of first aid measures

General advice

Consult a physician. Show this safety data sheet to the doctor in attendance.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

Extinguishing media

Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

Special hazards arising from the substance or mixture

Carbon oxides

Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

Further information

No data available

NFPA 704



HEALTH 2 Intense or continued but not chronic exposure could cause temporary incapacitation or possible residual injury (e.g. [diethyl ether](#), ammonium phosphate, iodine)

FIRE 1 Materials that require considerable preheating, under all ambient temperature conditions, before ignition and combustion can occur. Includes some finely divided suspended solids that do not require heating before ignition can occur. Flash point at or above 93.3 °C (200 °F). (e.g. [mineral oil](#), ammonia)

REACT 0 Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, [N₂](#))

SPEC.

HAZ.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation.

For personal protection see section 8.

Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

Methods and materials for containment and cleaning up

Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist. For precautions see section 2.2.

Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage. Store in cool place.

Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

control parameter

Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

Exposure controls

Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye/face protection

Safety glasses with side-shields conforming to EN166 Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

Body Protection

Impervious clothing, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full- face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Appearance light yellow clear, liquid

Odour No data available

Odour Threshold No data available

pH No data available

Melting point/freezing point	Melting point/freezing point: -40,37 °C
Initial boiling point and boiling range	98 - 99 °C at 12 hPa - lit.
Flash point	97 °C - closed cup
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	No data available
Vapour pressure	< 0,01 hPa at 20 °C
Vapour density	5,46 - (Air = 1.0)
Relative density	0,828 g/cm ³ at 20 °C
Water solubility	0,064 g/l at 20 °C
Partition coefficient: n-octanol/water	log Pow: 3,99 at 25 °C
Autoignition temperature	No data available
Decomposition temperature	No data available
Viscosity	No data available
Explosive properties	No data available
Oxidizing properties	No data available

Other safety information

Relative vapour density
5,46 - (Air = 1.0)

SECTION 10: Stability and reactivity

Reactivity

No data available

Chemical stability

Stable under recommended storage conditions.

Possibility of hazardous reactions

No data available

Conditions to avoid

No data available

Incompatible materials

Strong oxidizing agents

Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides Other decomposition products - No data available

In the event of fire: see section 5

SECTION 11: Toxicological information

Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - > 5.000 mg/kg LD50 Dermal - Rabbit - 2.400 mg/kg

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitisation

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

Additional Information

RTECS: RH0900000

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

SECTION 12: Ecological information

Toxicity

No data available

Toxicity to daphnia and other aquatic invertebrates

static test EC50 - Daphnia magna (Water flea) - 3,6 mg/l - 48 h

Persistence and degradability

Biodegradability aerobic - Exposure time 28 d

Result: 70 - 80 % - Not readily biodegradable. (OECD Test Guideline 301B)

Remarks: The 10 day time window criterion is not fulfilled.

Bioaccumulative potential

No data available

Mobility in soil

No data available

Results of PBT and vPvB assessment

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

Other adverse effects

Toxic to aquatic life with long lasting effects. No data available

SECTION 13: Disposal considerations

Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Waste material must be disposed of in accordance with the Directive on waste 2008/98/EC as well as other national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

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UN number

ADR/RID:IMDG:IATA:ADR/RID:IMDG:IATA:

UN number

ADR/RID:IMDG:IATA:ADR/RID:IMDG:IATA:

IATA:

UN number

ADR/RID: 3077 IMDG: 3077 IATA: 3077

ADR/RID: 1993 IMDG: 1993 IATA: 1993

ADR/RID: 3 (8) IMDG: 3 (8) IATA: 3 (8)

ADR/RID: 2585 IMDG: 2585 IATA: 2585

ADR/RID: - IMDG: - IATA: -

ADR/RID: 3272 IMDG: 3272 IATA: 3272

ADR/RID: 2937 IMDG: 2937 IATA: 2937

ADR/RID: 3271 IMDG: 3271 IATA: 3271

ADR/RID: - IMDG: - IATA: - UN proper shipping name ADR/RID: Not dangerous goods IMDG: Not dangerous goods IATA: Not dangerous goods

ADR/RID: 2987 IMDG: 2987 IATA: 2987

ADR/RID: - IMDG: - IATA: -

Packaging group

ADR/RID: - IMDG: - IATA: -

ADR/RID: CHLOROSILANES, CORROSIVE, N.O.S. IMDG: CHLOROSILANES, CORROSIVE, N.O.S. IATA: Chlorosilanes, corrosive, n.o.s.

Passenger Aircraft: Not permitted for transport

ADR/RID: - IMDG: - IATA: -

ADR/RID: ETHERS, N.O.S. (Diethyleneglycol dimethylether) IMDG: ETHERS, N.O.S. (Diethyleneglycol dimethylether) IATA: Ethers, n.o.s. (Diethyleneglycol dimethylether)

ADR/RID: alpha-METHYLBENZYL ALCOHOL, LIQUID IMDG: alpha-METHYLBENZYL ALCOHOL, LIQUID IATA: alpha-Methylbenzyl alcohol, liquid

ADR/RID: ESTERS, N.O.S. (Ethyl 3-methyl-2-oxobutyrate) IMDG: ESTERS, N.O.S. (Ethyl 3-methyl-2-oxobutyrate) IATA: Esters, n.o.s. (Ethyl 3-methyl-2-oxobutyrate)

ADR/RID: - IMDG: - IATA: -

ADR/RID: ARYLSULPHONIC ACIDS, SOLID IMDG: ARYLSULPHONIC ACIDS, SOLID IATA: Arylsulphonic acids, solid

ADR/RID: III IMDG: III IATA: III

ADR/RID: FLAMMABLE LIQUID, N.O.S. (3-Methylanisole) IMDG: FLAMMABLE LIQUID, N.O.S. (3-Methylanisole) IATA: Flammable liquid, n.o.s. (3-Methylanisole)

ADR/RID: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. ((1R,3S,4S)-N- Boc-2-azabicyclo[2.2.1]heptane-3-carboxylic acid) IMDG: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. ((1R,3S,4S)-N- IATA: Environmentally hazardous substance, solid, n.o.s. azabicyclo[2.2.1]heptane-3-carboxylic acid)

Transport hazard class(es)

((1R,3S,4S)-N-Boc-2- ADR/RID: 9 IMDG: 9 IATA: 9

ADR/RID: 3 IMDG: 3 IATA: 3

ADR/RID: no IMDG Marine pollutant: no IATA: no

ADR/RID: 8 IMDG: 8 IATA: 8

ADR/RID: no IMDG Marine pollutant: no IATA: no

ADR/RID: 3 IMDG: 3 IATA: 3

ADR/RID: 6.1 IMDG: 6.1 IATA: 6.1

ADR/RID: 3 IMDG: 3 IATA: 3

ADR/RID: - IMDG: - IATA: -

ADR/RID: 8 IMDG: 8 IATA: 8

ADR/RID: no IMDG Marine pollutant: no IATA: no

Special precautions for user

No data available

ADR/RID: II IMDG: II IATA: II

ADR/RID: no IMDG Marine pollutant: no IATA: no

ADR/RID: III IMDG: III IATA: III

ADR/RID: III IMDG: III IATA: III

ADR/RID: III IMDG: III IATA: III

No data available

ADR/RID: III IMDG: III IATA: III

No data available

ADR/RID: III IMDG: III IATA: III

Environmental hazards

ADR/RID: no IMDG Marine pollutant: no IATA: no Special precautions for user No data available

ADR/RID: no IMDG Marine pollutant: no IATA: no

ADR/RID: no IMDG Marine pollutant: no IATA: no

ADR/RID: no IMDG Marine pollutant: no IATA: no Special precautions for user No data available

ADR/RID: no IMDG Marine pollutant: no IATA: no

No data available

ADR/RID: no IMDG Marine pollutant: no IATA: no

Special precautions for user

No data available

No data available

No data available

No data available

SECTION 15: Regulatory information

Safety, health and environmental regulations/legislation specific for the substance or mixture

Regulations on the Safety Management of Hazardous Chemicals

China Catalog of Hazardous chemicals 2015:Not Listed. website: <https://www.mem.gov.cn/>

Measures for Environmental Management of New Chemical Substances

United States Toxic Substances Control Act (TSCA) Inventory:Listed. website: <https://www.epa.gov/>

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Listed. website: <https://emb.gov.ph/>

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Listed. website: <https://www.mee.gov.cn/>

EC Inventory:Listed.

New Zealand Inventory of Chemicals (NZIoC):Listed. website: <https://www.epa.govt.nz/>

European Inventory of Existing Commercial Chemical Substances (EINECS):Listed. website: <https://echa.europa.eu/>

Korea Existing Chemicals List (KECL):Listed. website: <http://ncis.nier.go.kr>

Vietnam National Chemical Inventory:Listed. website: <https://chemicaldata.gov.vn/>

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

References

- 【1】 CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>
- 【2】 ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>
- 【3】 ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>
- 【4】 eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:
http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en
- 【5】 ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>
- 【6】 Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>
- 【7】 HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>
- 【8】 IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>
- 【9】 IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>
- 【10】 Sigma-Aldrich, website: <https://www.sigmaaldrich.com/>

Disclaimer:

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