

Chemical Safety Data Sheet MSDS / SDS

DODECANE

Revision Date:2024-06-22 Revision Number:1

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

Product identifier

Product name : DODECANE
CBnumber : CB8678168
CAS : 93685-81-5
EINECS Number : 297-629-8
Synonyms : Heterogeneous cetane, Dihexyl

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

Classification of the substance or mixture

Flammable liquids, Category 3
Aspiration hazard, Category 1
Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 4

Label elements

Pictogram(s)

Signal word : Danger

Hazard statement(s)

H226 Flammable liquid and vapour
H304 May be fatal if swallowed and enters airways
H413 May cause long lasting harmful effects to aquatic life

Precautionary statement(s)

Prevention

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
Chemical Book

P233 Keep container tightly closed.

P240 Ground and bond container and receiving equipment.

P241 Use explosion-proof [electrical/ventilating/lighting/...] equipment.

P242 Use non-sparking tools.

P243 Take action to prevent static discharges.

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

P273 Avoid release to the environment.

Response

P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse affected areas with water [or shower].

P370+P378 In case of fire: Use ... to extinguish.

P301+P316 IF SWALLOWED: Get emergency medical help immediately.

P331 Do NOT induce vomiting.

Storage

P403+P235 Store in a well-ventilated place. Keep cool.

P405 Store locked up.

Disposal

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

Other hazards

no data available

SECTION 3: Composition/information on ingredients

Substance

Product name	: DODECANE
Synonyms	: Heterogeneous cetane, Dihexyl
CAS	: 93685-81-5
EC number	: 297-629-8
MF	: C ₁₂ H ₂₆
MW	: 170.33

SECTION 4: First aid measures

Description of first aid measures

If inhaled

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately.

Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

Following skin contact

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

Following eye contact

Rinse with pure water for at least 15 minutes. Consult a doctor.

Following ingestion

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison Control Center immediately.

Most important symptoms and effects, both acute and delayed

SYMPTOMS: Symptoms associated with exposure to aliphatic hydrocarbons may include nausea vomiting, dizziness, weakness, central nervous system effects such as depression, convulsions and, in extreme cases, coma. Other symptoms may include pulmonary and gastrointestinal irritation, pulmonary edema, bronchial pneumonia, anorexia, anemia, nervousness, pain in the limbs and numbness.

ACUTE/CHRONIC HAZARDS: Inhalation of this chemical may cause pulmonary irritation. It may also cause IMMEDIATELY leave the contaminated area; take deep breaths of fresh air. If symptoms (such as wheezing, coughing, shortness of breath, or burning in the mouth, throat, or chest) develop, call a physician and be prepared to transport the victim to a hospital. Provide proper respiratory protection to rescuers entering an unknown atmosphere. Whenever possible, Self-Contained Breathing Apparatus (SCBA) should be used; if not available, use a level of protection greater than or equal to that advised under Protective Clothing. (NTP, 1992)

Indication of any immediate medical attention and special treatment needed

Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR if necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on the left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. Aliphatic hydrocarbons and related compounds

SECTION 5: Firefighting measures

Extinguishing media

Suitable extinguishing media: Use water spray, alcohol-resistant foam, dry chemical, or carbon dioxide.

Specific Hazards Arising from the Chemical

This chemical is combustible. (NTP, 1992)

Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing mist, gas or vapours. Avoid contacting with skin and eye. Use personal protective equipment. Wear chemical impermeable gloves. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

Environmental precautions

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

Methods and materials for containment and cleaning up

ACCIDENTAL RELEASE MEASURES: Personal precautions, protective equipment and emergency procedures: Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapors accumulating to form explosive concentrations. Vapors can accumulate in low areas. Environmental precautions: Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Methods and materials for containment and cleaning up: Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations. Keep in suitable, closed containers for disposal.

SECTION 7: Handling and storage

Precautions for safe handling

Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

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. Handle and store under inert gas. Hygroscopic.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

no data available

Biological limit values

no data available

Exposure controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

Individual protection measures

Eye/face protection

Wear tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

Skin protection

Wear fire/flammable resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Physical state	PHYSICAL DESCRIPTION: Clear colorless liquid. (NTP, 1992)
Colour	Colorless liquid
Odour	no data available
Melting point/freezing point	-9.6°C(lit.)
Boiling point or initial boiling point and boiling range	215-217°C(lit.)
Flammability	no data available
Lower and upper explosion limit/flammability limit	Lower 0.6% by vol
Flash point	181.4 °F
Auto-ignition temperature	400° F (NTP, 1992)
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	Less than 32 SUS (Saybolt Universal Seconds)
Solubility	less than 1 mg/mL at 77° F (NTP, 1992)
Partition coefficient n-octanol/water	log Kow = 6.10
Vapour pressure	1 mm Hg (47.8 °C)
Density and/or relative density	0.75 g/mL at 25°C(lit.)
Relative vapour density	5.96 (vs air)
Particle characteristics	no data available

SECTION 10: Stability and reactivity

Reactivity

Flammable. Insoluble in water.

Chemical stability

Stable under recommended storage conditions.

Possibility of hazardous reactions

Combustible. Saturated aliphatic hydrocarbons, such as N-DODECANE, may be incompatible with strong oxidizing agents like nitric acid. Charring of the hydrocarbon may occur followed by ignition of unreacted hydrocarbon and other nearby combustibles. In other settings, aliphatic saturated hydrocarbons are mostly unreactive. They are not affected by aqueous solutions of acids, alkalis, most oxidizing agents, and most reducing agents. When heated sufficiently or when ignited in the presence of air, oxygen or strong oxidizing agents, they burn exothermically to produce carbon dioxide and water.

Conditions to avoid

no data available

Incompatible materials

Incompatible materials: Strong oxidizing agents.

Hazardous decomposition products

When heated to decomposition it emits acrid smoke and irritating fumes.

SECTION 11: Toxicological information

Acute toxicity

- Oral: no data available
- Inhalation: no data available
- Dermal: no data available

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

no data available

Reproductive toxicity

no data available

STOT-single exposure

no data available

STOT-repeated exposure

no data available

Aspiration hazard

no data available

SECTION 12: Ecological information

Toxicity

Toxicity to fish: no data available

Toxicity to daphnia and other aquatic invertebrates: no data available

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

Persistence and degradability

AEROBIC: Dodecane has been determined to be readily biodegradable based results of analogous chemicals incubated using an activated sludge inoculum in the Japanese MITI test(1). Thirty seven percent dodecane was mineralized in a 5-day biodegradability test using activated sludge with most of the remaining radioactivity from the labeled substrate being bound to the sludge as un-extractable residue(2). In other studies, 74% of the theoretical BOD was achieved in 24 hrs(3).

Bioaccumulative potential

A log BCF of 1.72 (BCF = 53) for golden orfes and a BCF of 50 for golden ide fish (*Leuciscus idus melanotus*) was determined for n-dodecane after 3 days exposure(1,2). An estimated BCF upper limit of <240 L/kg was calculated for dodecane in fathead minnows in water at concentrations less than its maximum aqueous solubility(3). According to a classification scheme(4), these BCF values suggest that bioconcentration in aquatic organisms is moderate to high(SRC). The bioaccumulation factor of n-dodecane in algae (*Chlorella fusca*) was determined to be 6,250 after 1 day(1); a log BCF of 3.80 for green algae after 24 hours exposure was also determined(1). Only traces of n-dodecane were taken up by a marine diatom from crude oil(5). The bioaccumulation factor of n-dodecane in activated sludge was determined to be 1,300 after 5 days(6).

Mobility in soil

Using a structure estimation method based on molecular connectivity indices(1), the Koc of dodecane can be estimated to be 4800(SRC). According to a classification scheme(2), this estimated Koc value suggests that dodecane is expected to have slight mobility in soil. In a study conducted to mimic a spill of 1.27 L/sq m, dodecane (present in JP-4 jet fuel) was transported to a depth of 10 cm; at the end of the study (134 days), it was no longer detected(3). In another study, it was determined that dodecane is slowly intercalated into well dried montmorillonite clay(4).

Other adverse effects

no data available

SECTION 13: Disposal considerations

Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

SECTION 14: Transport information

UN Number

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

Transport hazard class(es)

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

Packing group, if applicable

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

Environmental hazards

ADR/RID: No

IMDG: No

IATA: No

Special precautions for user

no data available

Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

Safety, health and environmental regulations specific for the product in question

European Inventory of Existing Commercial Chemical Substances (EINECS)

Listed.

EC Inventory

Listed.

United States Toxic Substances Control Act (TSCA) Inventory

Not Listed.

China Catalog of Hazardous chemicals 2015

Not Listed.

New Zealand Inventory of Chemicals (NZIoC)

Listed.

PICCS

Listed.

Vietnam National Chemical Inventory

Listed.

IECSC

Listed.

Korea Existing Chemicals List (KECL)

Listed.

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

IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>

HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: http://www.echemportal.org/echemportal/index?pagelD=0&request_locale=en

CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>

Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

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