Chemical Safety Data Sheet MSDS / SDS

Isodecanol

Revision Date: 2024-06-08 Revision Number: 1

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

Product identifier

Product name : Isodecanol
CBnumber : CB0751878
CAS : 68526-85-2
EINECS Number : 271-234-0
Synonyms : Isodecanol

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

Skin irritation, Category 2

Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 3 $\,$

Label elements

Pictogram(s)

Signal word Warning

Hazard statement(s)

H315 Causes skin irritation

H412 Harmful to aquatic life with long lasting effects

Precautionary statement(s)

Prevention

P264 Wash ... thoroughly after handling.

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

P273 Avoid release to the environment.

Response

P302+P352 IF ON SKIN: Wash with plenty of water/...

P321 Specific treatment (see ... on this label).

P332+P317 If skin irritation occurs: Get medical help.

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

Storage

none

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 : Isodecanol Synonyms : Isodecanol CAS : 68526-85-2 EC number : 271-234-0 : C10H22O MF : 158.28 MW

SECTION 4: First aid measures

Description of first aid measures

If inhaled

Fresh air, rest. Refer for medical attention.

Following skin contact

Remove contaminated clothes. Rinse and then wash skin with water and soap. Refer for medical attention .

Following eye contact

First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

Following ingestion

Rinse mouth. Rest. Refer for medical attention.

Most important symptoms and effects, both acute and delayed

Direct contact with skin can produce irritation. (USCG, 1999)

Indication of any immediate medical attention and special treatment needed

Basic Treatment: Establish a patent airway (oropharyngeal or nasopharyngeal airway, if needed). Suction if necessary. Watch for signs of respiratory insufficiency and assist ventilations if necessary. Administer oxygen by nonrebreather mask at 10 to 15 L/min. Monitor for shock Chemical Book

and treat if necessary . Monitor for pulmonary edema and treat if necessary . Anticipate seizures and treat if necessary . For eye contamination, flush eyes immediately with water. Irrigate each eye continuously with 0.9% saline (NS) during transport . Do not use emetics. For ingestion, rinse mouth and administer 5 ml/kg up to 200 ml of water for dilution if the patient can swallow, has a strong gag reflex, and does not drool. Administer activated charcoal . Higher alcohols (>3 carbons) and related compounds

SECTION 5: Firefighting measures

Extinguishing media

Extinguish with dry chemical, alcohol foam, or carbon dioxide. Water may be ineffective on fire.

Specific Hazards Arising from the Chemical

Excerpt from ERG Guide 171 [Substances (Low to Moderate Hazard)]: Some may burn but none ignite readily. Containers may explode when heated. Some may be transported hot. For UN3508, be aware of possible short circuiting as this product is transported in a charged state. (ERG, 2016)

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

Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

Methods and materials for containment and cleaning up

Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent and remove to safe place.

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

Separated from strong oxidants. Materials which are toxic as stored or which can decompose into toxic components ... should be stored in a cool well ventilated place, out of the direct rays of the sun, away from areas of high fire hazard, and should be periodically inspected.

Chemical Book

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 riskelimination 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/flame 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	Liquid. Moderate viscosity.
Colour	5 (Pt/Co) scale, colourless.
Odour	WEAK ALCOHOLIC
Melting point/freezing point	-78 °C. Atm. press.:1 013 hPa.
Boiling point or initial boiling point and	217 - 224 °C. Atm. press.:1 013 hPa.
boiling range	
Flammability	Combustible.
Lower and upper explosion	no data available
limit/flammability limit	
Flash point	99 °C. Atm. press.:1 013 hPa.
Auto-ignition temperature	280 °C. Atm. press.:1 013 hPa.
Decomposition temperature	no data available
рН	no data available

Kinematic viscosity	kinematic viscosity (in mm2/s) = 21. Temperature:20°C.
Solubility	Insoluble in water
Partition coefficient n-octanol/water	log Pow = 3.8. Temperature:25 °C. Remarks:Weighted log Pow (range 3.8-3.8).
Vapour pressure	1.1 kPa. Temperature:100 °C. Remarks:The value was calculated based on the extrapolation by
	Clausius-Clapeyron.
Density and/or relative density	0.838 g/cm3. Temperature:20 °C.
Relative vapour density	5.5 (AIR= 1)
Particle characteristics	no data available

SECTION 10: Stability and reactivity

Reactivity

Reacts with strong oxidants.

Chemical stability

no data available

Possibility of hazardous reactions

Combustible when exposed to heat or flame.ISODECYL ALCOHOL attacks plastics. REF [Handling Chemicals Safely, 1980. p. 236]. Acetyl bromide reacts violently with alcohols or water, [Merck 11th ed., 1989]. Mixtures of alcohols with concentrated sulfuric acid and strong hydrogen peroxide can cause explosions. Example: An explosion will occur if dimethylbenzylcarbinol is added to 90% hydrogen peroxide then acidified with concentrated sulfuric acid. Mixtures of ethyl alcohol with concentrated hydrogen peroxide form powerful explosives. Mixtures of hydrogen peroxide and 1-phenyl-2-methyl propyl alcohol tend to explode if acidified with 70% sulfuric acid, [Chem. Eng. News 45(43):73(1967); J, Org. Chem. 28:1893(1963)]. Alkyl hypochlorites are violently explosive. They are readily obtained by reacting hypochlorous acid and alcohols either in aqueous solution or mixed aqueous-carbon tetrachloride solutions. Chlorine plus alcohols would similarly yield alkyl hypochlorites. They decompose in the cold and explode on exposure to sunlight or heat. Tertiary hypochlorites are less unstable than secondary or primary hypochlorites, [NFPA 491 M, 1991]. Base-catalysed reactions of isocyanates with alcohols should be carried out in inert solvents. Such reactions in the absence of solvents often occur with explosive violence, [Wischmeyer(1969)].

Conditions to avoid

no data available

Incompatible materials

Reacts with strong oxidants.

Hazardous decomposition products

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

SECTION 11: Toxicological information

Acute toxicity

- Oral: LD50 rat (male) > 2 648 mg/kg bw.
- Inhalation: LC50 Swiss albino mice, Wistar rats, English short-hair quinea pigs > 95.3 ppm.

• Dermal: LD50 - rabbit (male/female) - > 3.16 mL/kg bw.

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: LC50 - Oncorhynchus mykiss (previous name: Salmo gairdneri) - 3.1 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: EL50 - Daphnia magna - 6.2 mg/L - 48 h.

Toxicity to algae: ChV - Green alga - 1.252 mg/L - 96 h.

Toxicity to microorganisms: no data available

Persistence and degradability

AEROBIC: In sewage, isodecyl alcohol gave a theoretical oxygen demand of 24, 44, 42 and 39 percent in 5, 10, 15 and 20 days, respectively(1). In acclimated sewage isodecyl alcohol gave theoretical oxygen demand of 14, 26, 45 and 32 percent in 5, 10, 15 and 20 days, respectively(1). Isodecyl alcohol gave theoretical oxygen demand of 6, 17, 34 and 40 percent in 5, 10, 15 and 20 days, respectively, in seawater(1). In a manometric study of poorly soluble compounds, isodecyl alcohol degraded 17.4 and 22.4 percent of ultimate BOD/theoretical oxygen demand with 10 minutes of sonification(2).

Bioaccumulative potential

An estimated BCF of 145 was calculated for isodecyl alcohol(SRC), using an estimated log Kow of 3.71(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is high(SRC), provided the compound is not metabolized by the organism(SRC).

Mobility in soil

Using a structure estimation method based on molecular connectivity indices(1), the Koc of isodecyl alcohol can be estimated to be 81(SRC). According to a classification scheme(2), this estimated Koc value suggests that isodecyl alcohol is expected to have high mobility in soil.

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

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?pageID=0&request_locale=en

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

ChemlDplus, 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/

Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.