ChemicalBook

Chemical Safety Data Sheet MSDS / SDS

ISOOCTYL ALCOHOL

Revision Date:2025-01-11 Revision Number:1

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

Product identifier

Product name	: ISOOCTYL ALCOHOL
CBnumber	: CB9506080
CAS	: 26952-21-6
EINECS Number	: 248-133-5
Synonyms	: Isoocityl alcohol,Isooctan-1-ol

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	: 010-86108875

SECTION 2: Hazards identification

Classification of the substance or mixture

Acute toxicity - Category 4, Oral

Skin irritation, Category 2

Eye irritation, Category 2

Label elements

Pictogram(s)

Signal word	Warning

Hazard statement(s)

H302 Harmful if swallowed

H315 Causes skin irritation

H319 Causes serious eye irritation

Precautionary statement(s)

Prevention

P264 Wash ... thoroughly after handling.

P270 Do not eat, drink or smoke when using this product.

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

Response

P301+P317 IF SWALLOWED: Get medical help.

P330 Rinse mouth.

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.

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

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	: ISOOCTYL ALCOHOL
Synonyms	: Isoocityl alcohol,Isooctan-1-ol
CAS	: 26952-21-6
EC number	: 248-133-5
MF	: C8H18O
MW	: 130.228

SECTION 4: First aid measures

Description of first aid measures

If inhaled

Fresh air, rest. Artificial respiration may be needed.

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. Give one or two glasses of water to drink. Refer for medical attention .

Most important symptoms and effects, both acute and delayed

Inhalation hazard slight. Skin contact results in moderate irritation. Liquid contact with eyes causes severe irritation and possible eye damage. (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 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

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SECTION 5: Firefighting measures

Extinguishing media

Extinguish with water, foam, dry chemical, or carbon dioxide, cool exposed containers with water.

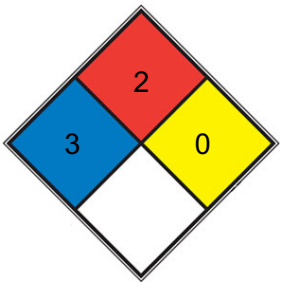
Specific Hazards Arising from the Chemical

Excerpt from ERG Guide 128 [Flammable Liquids (Water-Immiscible)]: HIGHLY FLAMMABLE: Will be easily ignited by heat, sparks or flames. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back. Most vapors are heavier than air. They will spread along ground and collect in low or confined areas (sewers, basements, tanks). Vapor explosion hazard indoors, outdoors or in sewers. Those substances designated with a (P) may polymerize explosively when heated or involved in a fire. Runoff to sewer may create fire or explosion hazard. Containers may explode when heated. Many liquids are lighter than water. Substance may be transported hot. For hybrid vehicles, ERG Guide 147 (lithium ion batteries) or ERG Guide 138 (sodium batteries) should also be consulted. If molten aluminum is involved, refer to ERG Guide 169. (ERG, 2016)

Advice for firefighters

Use powder, carbon dioxide, foam.

NFPA 704



HEALTH	3	Short exposure could cause serious temporary or moderate residual injury (e.g. liquid hydrogen, sulfuric acid, calcium hypochlorite, hexafluorosilicic acid)
FIRE	2	Must be moderately heated or exposed to relatively high ambient temperature before ignition can occur and multiple finely divided suspended solids that do not require heating before ignition can occur. Flash point between 37.8 and 93.3 °C (100 and 200 °F). (e.g. diesel fuel, sulfur)
REACT	0	Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium,N2)

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SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Ventilation. 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.

Environmental precautions

Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Ventilation. 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

Ventilation. 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

NO open flames. Above 82°C use a closed system and ventilation. 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.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

TLV: 50 ppm as TWA; (skin)

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 safety goggles.

Skin protection

Protective gloves.

Respiratory protection

Use ventilation.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Physical state	Liquid; a mixture of closely related isomeric, primary alcohols with branched chains
Colour	Clear, colorless liquid.
Odour	Mild
Melting point/freezing point	<-76°C
Boiling point or initial boiling point and boiling range	179.2°C at 760 mmHg
Flammability	Class IIIA Combustible Liquid: Fl.P. at or above 140°F and below 200°F.
Lower and upper explosion limit/flammability limit	Lower flammable limit: 0.9% by volume
Flash point	71.1°C
Auto-ignition temperature	530° F (USCG, 1999)
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	10.6 centipoise at 15 deg C
Solubility	Insoluble (NIOSH, 2016)
Partition coefficient n-octanol/water	log Kow = 2.73 (est)
Vapour pressure	1.03 mm Hg (USCG, 1999)
Density and/or relative density	0.821 g/cm3
Relative vapour density	(air = 1): 4.5
Particle characteristics	no data available

SECTION 10: Stability and reactivity

Reactivity

Reacts with strong oxidants.

Reacts violently with strong oxidants and strong bases. Decomposes on heating and on burning.

Chemical stability

no data available

Possibility of hazardous reactions

ISOOCTYL 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 oral 1.5 g/kg
- 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

The substance is irritating to the eyes, skin and respiratory tract. The substance may cause effects on the central nervous system.

STOT-repeated exposure

The substance defats the skin, which may cause dryness or cracking.

Aspiration hazard

A harmful contamination of the air will not or will only very slowly be reached on evaporation of this substance at 20°C.

SECTION 12: Ecological information

Toxicity

Toxicity to fish: LC50 Lepomis macrochirus (Bluegill) 30 mg/L/24 hr, static
Toxicity to daphnia and other aquatic invertebrates: EC50 Daphnia magna (Water flea; intoxication, immobilization) 115 mg/L/24 hr; static /formulated product
Toxicity to algae: EC50 Scenedesmus subspicatus (Green algae; cell multiplication inhibition) 14 mg/L/48 hr; static /formulated product
Toxicity to microorganisms: no data available

Persistence and degradability

Data regarding the biodegradation of isooctyl alcohol were not available(SRC, 2006). Yet, a number of aerobic and anaerobic biological screening studies, which utilized settled waste water, sewage, or activated sludge for inocula, have demonstrated that n-octanol is biodegradable(1-9). Since isooctyl alcohol is a mixture of isomers where most of the molecule is a straight chain alcohol, the results of the studies on n-octanol would suggest rapid biodegradation where acclimation has occurred(SRC).

Bioaccumulative potential

An estimated BCF of 16 was calculated for isooctyl alcohol(SRC), using a water solubility of 640 mg/L(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

Mobility in soil

The Koc of isooctyl alcohol is estimated as 125(SRC), using a water solubility of 640 mg/L(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that isooctyl alcohol is expected to have high mobility in soil.

Toxics Screening Level

The initial threshold screening level (ITSL) for isooctanol (also called isooctyl alcohol) is 2700 µg/m3 (8-hour averaging time).

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: UN3082 (For reference only, please check.)

IMDG: UN3082 (For reference only, please check.)

IATA: UN3082 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (For reference only, please check.)

IMDG: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (For reference only, please check.)

IATA: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (For reference only, please check.)

Transport hazard class(es)

ADR/RID: 9 (For reference only, please check.)

IMDG: 9 (For reference only, please check.)

IATA: 9 (For reference only, please check.)

Packing group, if applicable

ADR/RID: III (For reference only, please check.)

IMDG: III (For reference only, please check.)

IATA: III (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

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/