Chemical Safety Data Sheet MSDS / SDS

Allyl alcohol SDS

Revision Date:2024-04-25 Revision Number:1

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

Product identifier

Product name: Allyl alcohol

CAS: 107-18-6

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.in

Address: 5 vasavi Layout Basaveswara Nilayam Pragathi Nagar Hyderabad, India -500090

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SECTION 2: Hazards identification

Classification of the substance or mixture

Flammable liquids, Category 2
Acute toxicity - Category 3, Oral

Acute toxicity - Category 3, Dermal
Skin irritation, Category 2
Eye irritation, Category 2
Acute toxicity - Category 3, Inhalation
Specific target organ toxicity – single exposure, Category 3
Hazardous to the aquatic environment, short-term (Acute) - Category Acute 1

GHS label elements, including precautionary statements

Pictogram(s)

Signal word Danger

Hazard statement(s)

H225 Highly flammable liquid and vapour
H301 Toxic if swallowed
H311 Toxic in contact with skin
H315 Causes skin irritation
H319 Causes serious eye irritation
H331 Toxic if inhaled
H335 May cause respiratory irritation
H400 Very toxic to aquatic life

Precautionary statement(s)

Prevention

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
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/...
P264 Wash ... thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P271 Use only outdoors or in a well-ventilated area.
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.
P321 Specific treatment (see ... on this label).
P330 Rinse mouth.
P302+P352 IF ON SKIN: Wash with plenty of water/...
P316 Get emergency medical help immediately.
P361+P364 Take off immediately all contaminated clothing and wash it before reuse.
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.
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P319 Get medical help if you feel unwell.
P391 Collect spillage.

Storage

P403+P235 Store in a well-ventilated place. Keep cool.
P405 Store locked up.
P403+P233 Store in a well-ventilated place. Keep container tightly closed.

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 which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

Substance

Chemical name:	Allyl alcohol
Common names and synonyms:	Allyl alcohol

CAS number:	107-18-6
EC number:	203-470-7
Concentration:	100%

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Fresh air, rest.

Following skin contact

Remove contaminated clothes. Rinse and then wash skin with water and soap.

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. Induce vomiting (ONLY IN CONSCIOUS PERSONS!). Rest. Refer for medical attention .

Most important symptoms/effects, acute and delayed

Allyl alcohol is an intense irritant to skin, eyes, nose, and throat. It causes burns on contact, and may cause pulmonary edema if inhaled. It is poisonous in small quantities. The probable oral lethal dose is 50-500 mg/kg, or between 1 teaspoonful and 1 ounce for a 150-lb. person. (EPA, 1998)

Indication of immediate medical attention and special treatment needed, if necessary

Inhibitors of alcohol dehydrogenase prevent periportal liver necrosis in animals treated with allyl alcohol.

SECTION 5: Firefighting measures

Suitable extinguishing media

Use water spray, dry chemical, "alcohol resistant" foam, or carbon dioxide. Water may be ineffective. Use water spray to keep

fire-exposed containers cool.

Specific hazards arising from the chemical

Allyl alcohol vapor may explode if ignited in confined areas. Combustion products may be poisonous. The vapor is heavier than air and flashback along vapor trail may occur. Gives off toxic fumes when heated. May react vigorously with oxidizing materials, carbon tetrachloride, acids, oleum, sodium hydroxide, diallyl phosphite, potassium chloride, or tri-n-bromomelamine. (EPA, 1998)

Special protective actions for fire-fighters

Use water in large amounts, powder, alcohol-resistant foam, carbon dioxide. In case of fire: keep drums, etc., cool by spraying with water.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Personal protection: complete protective clothing including self-contained breathing apparatus. Remove all ignition sources. Do NOT let this chemical enter the environment. 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: complete protective clothing including self-contained breathing apparatus. Remove all ignition sources. Do NOT let this chemical enter the environment. 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

Releases may require isolation or evacuation. Stop or control the leak, if this can be done without undue risk. Use water spray to cool and disperse vapors, protect personnel, and dilute spills to form nonflammable mixtures. Approach release from upwind. Eliminate all ignition sources. Control runoff and isolate discharged material for proper disposal.

SECTION 7: Handling and storage

Precautions for safe handling

NO open flames, NO sparks and NO smoking. Above 21°C use a closed system, ventilation and explosion-proof electrical equipment. 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

Fireproof. Separated from strong oxidants and food and feedstuffs.Separate from oxidizing materials. Store in a dry, cool, well-ventilated location.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

TLV: 0.5 ppm as TWA; (skin); A4 (not classifiable as a human carcinogen).EU-OEL: 4,8 mg/m3, 2 ppm as TWA; 12,1 mg/m3, 5 ppm as STEL; (skin).MAK: skin absorption (H); carcinogen category: 3B

Biological limit values

no data available

Appropriate engineering 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, such as personal protective equipment (PPE)

Eye/face protection

Wear face shield or eye protection in combination with breathing protection.

Skin protection

Protective gloves. Protective clothing.

Respiratory protection

Use ventilation, local exhaust or breathing protection.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state:	Liquid. Allyl alcohol is a liquid.
Colour:	Colourless.
Odour:	Pungent, mustard-like odor
Melting point/freezing point:	-129 °C.
Boiling point or initial boiling point and boiling range:	97.4 °C. Atm. press.: 101.3 kPa.
Flammability:	Class IB Flammable Liquid: Fl.P. below 73°F and BP at or above 100°F.
Lower and upper explosion limit/flammability limit:	Lower flammable limit: 2.5% by volume; Upper flammable limit: 18.0% by volume
Flash point:	21 °C. Atm. press.: 101.3 kPa.
Auto-ignition temperature:	713 °F. Remarks: Reported value is assumed to have been determined at STP (20 degrees C, 101.3 kPa).
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	dynamic viscosity (in mPa s) = < 10. Temperature: 20°C.; dynamic viscosity (in mPa s) = < 10. Temperature: 40°C.
Solubility:	Miscible (NIOSH, 2016)
Partition coefficient n-octanol/water:	log Pow = 0.21.
Vapour pressure:	31.12 hPa. Temperature: 25 °C. Remarks: Mean vapour pressure from Antoine and Grain methods using the MPBPVP v1.43 module of EPISuite v4.0.
Density and/or relative density:	0.854. Temperature: 20 °C.

Relative vapour density:	2 (vs air)
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

Reacts with carbon tetrachloride, nitric acid and chlorosulfonic acid. This generates fire and explosion hazard.

Chemical stability

Upon storage for several years allyl alcohol polymerizes and a thick syrup is formed (insol in water, sol in chloroform) which on treatment with ether yields a brittle resinoid mass.

Possibility of hazardous reactions

AT 22 DEG C, LIQUID GIVES OFF FLAMMABLE CONCN OF VAPOR IN AIR. ALLYL ALCOHOL presents a dangerous fire and explosion hazard when exposed to heat, flame, or oxidizing agents. Reacts violently or explosively with sulfuric acid, strong bases. Reacts violently with 2,4,6-trichloro-1,3,5-triazine and 2,4,6-tris(bromoamino)-1,3,5-triazine. Reacts with carbon tetrachloride to produce explosively unstable products [Lewis]. Mixing allyl alcohol in equal molar portions with any of the following substances in a closed container caused the temperature and pressure to increase: chlorosulfonic acid, nitric acid, oleum, sulfuric acid [NFPA 491M. 1991].

Conditions to avoid

no data available

Incompatible materials

A reaction between allyl alcohol and carbon tetrachloride produced trichlorobutylene epoxide (oxide) and dichlorobutylene epoxide (oxide), a mixture which during distillation proved to be unstable and detonated in the still.

Hazardous decomposition products

Energy of decomposition (in range 360-500 deg C) measured as 0.69 kJ/g.

SECTION 11: Toxicological information

Acute toxicity

Oral: LD50 - rat (male) - 105 mg/kg bw. Remarks:For animals weighing 111-143 g.

Inhalation: LC50 - rat (male/female) - > 100 ppm.

Dermal: LD50 - rabbit (male) - 89 mg/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

A4; Not classifiable as a human carcinogen.

Reproductive toxicity

no data available

STOT-single exposure

Lachrymation. The substance is irritating to the eyes, skin and respiratory tract. The substance may cause effects on the muscles. This may result in local spasm and aching. The effects may be delayed. The substance may cause effects on the kidneys and liver.

STOT-repeated exposure

no data available

Aspiration hazard

A harmful contamination of the air can be reached very quickly on evaporation of this substance at 20°C.

SECTION 12: Ecological information

Toxicity

Toxicity to fish: LC50 - Pimephales promelas - 0.32 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: EC50 - Daphnia magna - 1.65 mg/L - 48 h.

Toxicity to algae: EC50 - Pseudokirchneriella subcapitata (previous names: Raphidocelis subcapitata, Selenastrum capricornutum) - 2.25 mg/L - 72 h.

Toxicity to microorganisms: IC50 - Tetrahymena pyriformis - 82.755 mmol/L - 2 d.

Persistence and degradability

AEROBIC: Allyl alcohol, present at 100 mg/L, reached 86% of its theoretical BOD in 2 weeks using an activated sludge inoculum at 30 mg/L in the Japanese MITI test which classified allyl alcohol as readily biodegradable(1). Following incubation of 20 deg C with settled sewage seed, 2.5 ppm of allyl alcohol had degraded to 9.1, 55.0, 78.2, and 81.8% of the theoretical BOD after 5, 10, 15, and 20 days, respectively(2). In a 5 day BOD test, 81% of the theoretical oxygen demand was observed following incubation of allyl alcohol at 20 deg C with a sewage seed(3). Allyl alcohol (25 ppm) was found to degrade 100 and 60% in marine and river water after 3 days at 30 deg C, respectively(4). Half-lives of 10.2 and 9.5 days at 20 deg C were found for allyl alcohol with Texas soil (pH 7.8, 3.25% organic matter) and Mississippi soil (pH 4.8, <1% organic matter), respectively(5).

Bioaccumulative potential

An estimated BCF of 3 in fish was calculated for allyl alcohol(SRC), using a log Kow of 0.17(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). The uptake of (14)C-allyl alcohol residues by lettuce and carrots was investigated in the greenhouse(4); uptake of residues was higher by carrots than by lettuce, and higher by lettuce roots than by lettuce tops(4); no bioaccumulation was observed(4).

Mobility in soil

Using a structure estimation method based on molecular connectivity indices(1), the Koc for allyl alcohol can be estimated to be 2(SRC). According to a classification scheme(2), this estimated Koc value suggests that allyl alcohol is expected to have very high mobility in soil. Leaching of allyl alcohol from soil surface to deeper layers was found to rank in order of sand > sandy loam > humus sand(3). The percent leached after 2 days and 400 mL of water with sand containing 0.51% and 2.89% organic matter were 100 and 83.3%, respectively(3). Freundlich adsorption coefficients for allyl alcohol in Texas soil (pH 7.8, 3.25% organic matter) and

Mississippi soil (pH 4.8, <1% organic matter) were 4.5X10-3 and 3.3X10-4, respectively(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: UN1098 (For reference only, please check.)
IMDG: UN1098 (For reference only, please check.)
IATA: UN1098 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: ALLYL ALCOHOL (For reference only, please check.)
IMDG: ALLYL ALCOHOL (For reference only, please check.)
IATA: ALLYL ALCOHOL (For reference only, please check.)

Transport hazard class(es)

ADR/RID: 6.1 (For reference only, please check.)
IMDG: 6.1 (For reference only, please check.)
IATA: 6.1 (For reference only, please check.)

Packing group, if applicable

ADR/RID: I (For reference only, please check.)
IMDG: I (For reference only, please check.)
IATA: I (For reference only, please check.)

Environmental hazards

ADR/RID: Yes
IMDG: Yes
IATA: Yes

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

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/

Other Information

Depending on the degree of exposure, periodic medical examination is suggested. The odour warning when the exposure limit value is exceeded is insufficient.