Chemical Safety Data Sheet MSDS / SDS

Allyl chloroformate 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 chloroformate

CAS: 2937-50-0

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

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SECTION 2: Hazards identification

Classification of the substance or mixture

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

Skin corrosion, Sub-category 1B
Acute toxicity - Category 1, Inhalation

GHS label elements, including precautionary statements

Pictogram(s)

Signal word Danger

Hazard statement(s)

H226 Flammable liquid and vapour
H301 Toxic if swallowed
H314 Causes severe skin burns and eye damage
H330 Fatal if inhaled

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.
P260 Do not breathe dust/fume/gas/mist/vapours/spray.
P271 Use only outdoors or in a well-ventilated area.
P284 [In case of inadequate ventilation] wear respiratory protection.

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.
P301+P330+P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

P363 Wash contaminated clothing before reuse.
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P316 Get emergency medical help immediately.
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P320 Specific treatment is urgent (see ... on this label).

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 chloroformate
Common names and synonyms:	Allyl chloroformate
CAS number:	2937-50-0
EC number:	220-916-6
Concentration:	100%

SECTION 4: First aid measures

Description of necessary 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/effects, acute and delayed

Vapor irritates eyes and respiratory tract. Contact with liquid causes eye and skin irritation, and ingestion irritates mouth and stomach. (USCG, 1999)

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

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 as necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on 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. Organic acids and related compounds

SECTION 5: Firefighting measures

Suitable extinguishing media

Use dry chemical, foam, carbon dioxide, or water spray. Water may be ineffective. Use water spray to keep fire-exposed containers cool. Approach fire from upwind to avoid hazardous vapors and toxic decomposition products.

Specific hazards arising from the chemical

Special Hazards of Combustion Products: When heated to decomposition, emits highly toxic phosgene gas. Behavior in Fire: Vapor is heavier than air and may travel considerable distance to a source of ignition and flash back. (USCG, 1999)

Special protective actions for fire-fighters

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

If material not in fire and not involved in fire: Neutralize spilled material with crushed limestone, soda ash, or lime.

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

Separate from acids, alkalies, amines, alcohols, oxidizing materials, water, & explosives. Store in a cool, dry, well-ventilated location. Normally refrigerated. Outside or detached storage is preferred.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

no data available

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 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 and safety characteristics

Physical state:	Allyl chlorocarbonate is a colorless liquid with a pungent odor. Flash point 88°F. Corrosive to metals and tissue. Very toxic by inhalation, ingestion and/or skin contact. Vapors are heavier than air.
Colour:	Hygroscopic liquid
Odour:	Pungent odor
Melting point/freezing point:	9°C(lit.)

Boiling point or initial boiling point and boiling range:	~27°C/11mmHg(lit.)
Flammability:	no data available
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	31°C
Auto-ignition temperature:	no data available
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	0.71 mPa-s (cP) at 20 deg C
Solubility:	Insoluble in water
Partition coefficient n-octanol/water:	log Kow = 0.98 (est)
Vapour pressure:	3.67 psi (20 °C)
Density and/or relative density:	1.134g/mLat 20°C(lit.)
Relative vapour density:	4.2 (Air = 1)
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

Highly flammable. Water reaction produces heat and acidic HCl. In the presence of moist air, corrosive hydrogen chloride is

produced.

Chemical stability

no data available

Possibility of hazardous reactions

Dangerous when exposed to heat, open flame (or sparks), or powerful oxidizers.Acid halides, such as ALLYL CHLOROCARBONATE, are water reactive; some are violently reactive. They are incompatible with strong oxidizing agents, alcohols, amines, alkali. May react vigorously or explosively if mixed with diisopropyl ether or other ethers in the presence of trace amounts of metal salts [J. Haz. Mat., 1981, 4, 291].

Conditions to avoid

no data available

Incompatible materials

Reacts with water to produce chloroformic acid & allyl alcohol.

Hazardous decomposition products

When heated to decomposition it emits toxic fumes of /chlorine/.

SECTION 11: Toxicological information

Acute toxicity

Oral: LD50 rats oral 244 mg/kg

Inhalation: LC50 Rat inhalation 32,400 ug/cu m

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

no data available

Bioaccumulative potential

An estimated BCF of 3 was calculated in fish for allyl chloroformate(SRC), using an estimated log Kow of 0.98(1) and a regression-derived equation(1). According to a classification scheme(2), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC). In addition, allyl chloroformate hydrolyzes rapidly in water(3) to form allyl alcohol and chloroformic acid(4) indicating bioconcentration is not an important environmental fate process(SRC).

Mobility in soil

Using a structure estimation method based on molecular connectivity indices(1), the Koc of allyl chloroformate can be estimated to be 5(SRC). According to a classification scheme(2), this estimated Koc value suggests that allyl chloroformate is expected to have very high mobility in soil. Allyl chloroformate hydrolyzes rapidly in water(3) to form allyl alcohol and chloroformic acid(4). Therefore, hydrolysis in moist soils will attenuate or eliminate the importance of environmental leaching(SRC).

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: UN1722 (For reference only, please check.)
IMDG: UN1722 (For reference only, please check.)
IATA: UN1722 (For reference only, please check.)

UN Proper Shipping Name

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

Listed.

New Zealand Inventory of Chemicals (NZIoC)

Listed.

(PICCS)

Listed.

Vietnam National Chemical Inventory

Listed.

IECSC)

Not Listed.

Korea Existing Chemicals List (KECL)

Not 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/