

Chemical Safety Data Sheet MSDS / SDS

2-propylvaleric acid SDS

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

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

Product name: 2-propylvaleric acid

CAS: 99-66-1

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**

Acute toxicity - Category 4, Oral

Skin irritation, Category 2

Serious eye damage, Category 1
Reproductive toxicity, Category 1A

GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Danger

Hazard statement(s)

H302 Harmful if swallowed
H315 Causes skin irritation
H318 Causes serious eye damage
H360 May damage fertility or the unborn child

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/...
P203 Obtain, read and follow all safety instructions before use.

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+P354+P338 IF IN EYES: Immediately rinse with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P317 Get medical help.
P318 IF exposed or concerned, get medical advice.

Storage

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 which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

Substance

Chemical name: 2-propylvaleric acid

Common names and synonyms: 2-propylvaleric acid

CAS number: 99-66-1

EC number: 202-777-3

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

SYMPTOMS: Symptoms of exposure to this compound may include gastrointestinal disturbances, hair loss, psychosis, altered bleeding time, altered liver enzymes and fatal hepatic failure. Other symptoms may include central nervous system depression, nausea, vomiting, indigestion, diarrhea, abdominal cramps, constipation, anorexia with weight loss, increased appetite with weight gain, tremor, ataxia, headache, nystagmus, diplopia, asterixis, spots before the eyes, dysarthria, dizziness, incoordination, coma, skin rash, erythema multiforme, generalized pruritus, emotional upset, depression, hyperactivity, behavioral deterioration, weakness, thrombocytopenia, petechiae, bruising, hematoma formation, frank hemorrhage, relative lymphocytosis, hypofibrinogenemia, leukopenia, eosinophilia, anemia, bone marrow suppression, irregular menses, secondary amenorrhea and breast enlargement. Changes in exocrine pancreas and sleep disturbances may also occur. It may also cause somnolence.

ACUTE/CHRONIC HAZARDS: When heated to decomposition this compound may emit toxic fumes of carbon monoxide and carbon dioxide. (NTP, 1992)

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

Administration of high-dose naloxone has been reported to reverse valproate-induced CNS depression. Theories regarding the reversal of sedation by naloxone include reversal of the release of endogenous opioids and reversal of valproate blockade of GABA uptake by cells. Serum glucose, calcium, phosphate, and platelets must be frequently measured and treated accordingly.

SECTION 5: Firefighting measures

Suitable extinguishing media

Fires involving this material can be controlled with a dry chemical, carbon dioxide or Halon extinguisher. (NTP, 1992)

Specific hazards arising from the chemical

This chemical is combustible. (NTP, 1992)

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

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

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

Store between 15 and 30 deg C (59 and 86 deg F), in a tight container. Valproic Acid Capsules USP

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/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 and safety characteristics

Physical state:	Liquid. Viscous.
Colour:	Colourless to pale yellow.
Odour:	Characteristic odor
Melting point/freezing point:	223°C(dec.)(lit.)
Boiling point or initial boiling point and boiling range:	Ca. 222 °C. Atm. press.:Ca. 760 mm Hg. Remarks:No data regarding decomposition.
Flammability:	no data available
Lower and upper explosion limit/flammability limit:	no data available

Flash point:	111°C
Auto-ignition temperature:	no data available
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	no data available
Solubility:	less than 1 mg/mL at 72° F (NTP, 1992)
Partition coefficient n-octanol/water:	no data available
Vapour pressure:	8.47X10 ⁻² mm Hg at 25 deg C (est)
Density and/or relative density:	0.9g/mL at 25°C (lit.)
Relative vapour density:	no data available
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

no data available

Chemical stability

no data available

Possibility of hazardous reactions

VALPROIC ACID is a carboxylic acid. Carboxylic acids donate hydrogen ions if a base is present to accept them. They react in this way with all bases, both organic (for example, the amines) and inorganic. Their reactions with bases, called "neutralizations", are

accompanied by the evolution of substantial amounts of heat. Neutralization between an acid and a base produces water plus a salt. Carboxylic acids with six or fewer carbon atoms are freely or moderately soluble in water; those with more than six carbons are slightly soluble in water. Soluble carboxylic acid dissociate to an extent in water to yield hydrogen ions. The pH of solutions of carboxylic acids is therefore less than 7.0. Many insoluble carboxylic acids react rapidly with aqueous solutions containing a chemical base and dissolve as the neutralization generates a soluble salt. Carboxylic acids in aqueous solution and liquid or molten carboxylic acids can react with active metals to form gaseous hydrogen and a metal salt. Such reactions occur in principle for solid carboxylic acids as well, but are slow if the solid acid remains dry. Even "insoluble" carboxylic acids may absorb enough water from the air and dissolve sufficiently in it to corrode or dissolve iron, steel, and aluminum parts and containers. Carboxylic acids, like other acids, react with cyanide salts to generate gaseous hydrogen cyanide. The reaction is slower for dry, solid carboxylic acids. Insoluble carboxylic acids react with solutions of cyanides to cause the release of gaseous hydrogen cyanide. Flammable and/or toxic gases and heat are generated by the reaction of carboxylic acids with diazo compounds, dithiocarbamates, isocyanates, mercaptans, nitrides, and sulfides. Carboxylic acids, especially in aqueous solution, also react with sulfites, nitrites, thiosulfates (to give H₂S and SO₃), dithionites (SO₂), to generate flammable and/or toxic gases and heat. Their reaction with carbonates and bicarbonates generates a harmless gas (carbon dioxide) but still heat. Like other organic compounds, carboxylic acids can be oxidized by strong oxidizing agents and reduced by strong reducing agents. These reactions generate heat. A wide variety of products is possible. Like other acids, carboxylic acids may initiate polymerization reactions; like other acids, they often catalyze (increase the rate of) chemical reactions. This chemical is incompatible with bases, oxidizing agents and reducing agents. It is corrosive. (NTP, 1992).

Conditions to avoid

no data available

Incompatible materials

no data available

Hazardous decomposition products

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

SECTION 11: Toxicological information**Acute toxicity**

Oral: LD50 Guinea pig oral 824 mg/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

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 valproic acid(SRC), using a log Kow of 2.75(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 valproic acid is estimated as 47(SRC), using a log Kow of 2.75(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that valproic acid is expected to have very high mobility in soil. The pKa of valproic acid is 4.6(4), indicating that this compound will exist almost entirely in the anion form in the environment and anions generally do not adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts(5).

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)

Not 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/>

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