Propylene glycol

Propylene glycol (IUPAC name: **propane-1,2-diol**) is a synthetic <u>organic compound</u> with the <u>chemical formula</u> $C_3H_8O_2$. It is a viscous, colorless liquid which is nearly odorless but possesses a faintly sweet taste. Chemically it is classed as a <u>diol</u> and is <u>miscible</u> with a broad range of solvents, including <u>water</u>, <u>acetone</u>, and chloroform.

It is produced on a large scale and is primarily used in the production of <u>polymers</u>, but also sees use in food processing, and as a process fluid in low-temperature heat-exchange applications. In the European Union, it has the <u>E-number</u> E1520 for food applications. For cosmetics andpharmacology, the number is E490.

The compound is sometimes called (alpha) α -propylene glycol to distinguish it from the isomerpropane-1,3-diol, known as (beta) β -propylene glycol.

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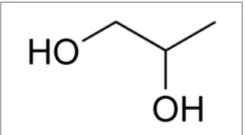
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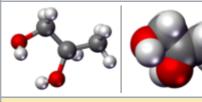
Structure and properties

Propylene glycol is a clear, colorless and <u>hygroscopic</u> liquid. Propylene glycol contains an asymmetrical <u>carbon atom</u>, so it exists in two <u>enantiomers</u>. The commercial product is a <u>racemic</u> mixture. Pure optical isomers can be obtained by hydration of optically pure propylene oxide [4]

The <u>freezing point</u> of water is depressed when mixed with propylene glycol, owing to the effects of dissolution of a solute in a solvent (<u>freezing-point depression</u>). In general, glycols are non-corrosive, have very low volatility and very low toxicity; however, the closely related <u>ethylene glycol</u> (a key ingredient in <u>antifreeze</u>) is toxic to humans and to many animals^[5]

Propylene glycol [1]





Names

Preferred IUPAC name Propane-1,2-diol

Other names

Propylene glycol

α-Propylene glycol

1,2-Propanediol

1,2-Dihydroxypropane

Methyl ethyl glycol (MEG)

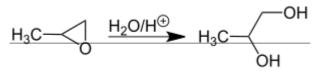
Methylethylene glycol

Identifiers	
CAS Number	57-55-6 ✓
3D model (JSmol)	Interactive image
ChEBI	CHEBI:16997 ✓
ChEMBL	ChEMBL286398 ✓
ChemSpider	13835224 🗸
ECHA	100.000.307
InfoCard	
EC Number	200-338-0
E number	E1520 (additional
	chemicals)
PubChem <u>CID</u>	1030
RTECS	TY6300000
number	
UNII	6DC9Q167V3 ✓
InChI	

Production

Industrial

Industrially, propylene glycol is produced from <u>propylene oxide [6]</u> (for food-grade use), and global capacity in 1990 was 900,000 tonnes per year. Different manufacturers use either non-catalytic high-temperature process at 200 °C (392 °F) to 220 °C (428 °F), or a catalytic method, which proceeds at 150 °C (302 °F) to 180 °C (356 °F) in the presence of ion exchange resin or a small amount of sulfuric acid or alkali.



Final products contain 20% propylene glycol, 1.5% of dipropylene glycol and small amounts of other polypropylene glycols. [8] Further purification produces finished industrial grade or USP/JP/EP/BP grade propylene glycol that is typically 99.5% or greater. Propylene glycol can also be converted from glycerol, a biodiesel byproduct. This starting material is usually reserved for industrial use because of the noticeable odor and taste that accompanies the final product.

Laboratory

 $\underline{\textit{S-Propanediol}}$ may be synthesized from $\underline{\textit{D-mannitol}}$, through the following scheme: [9]

SMILES		
Р	roperties	
Chemical formula	C ₃ H ₈ O ₂	
Molar mass	76.10 g·mol ⁻¹	
Density	1.036 g/cm ³	
Melting point	−59 °C (−74 °F; 214 K)	
Boiling point	188.2 °C (370.8 °F; 461.3 K)	
Solubility in water	Miscible	
Solubility in ethanol	Miscible	
Solubility in diethyl ether	Miscible	
Solubility in acetone	Miscible	
Solubility in chloroform	Miscible	
log P	-1.34 ^[2]	
Thermal	0.34 W/m-K (50%	
conductivity	H ₂ O @ 90 °C	
	(194 °F))	
Viscosity	0.042 Pa·s	
Pharmacology		
ATCvet code	QA16QA01 (WHO)	
ا	Hazards	
S-phrases (outdated)	<u>S24 S25</u>	
NFPA 704	0 1 0	
Related compounds		
Related glycols	Ethylene glycol, 1,3- propanediol	
Except where otherwise noted, data are given for materials in their standard state (at 25 °C [77 °F], 100 kPa).		
✓ verify (what is 👫 ?) Infobox references		

Applications

Forty-five percent of propylene glycol produced is used as chemical feedstock for the production of unsaturated polyester resins. In this regard, propylene glycol reacts with a mixture of unsaturated maleic anhydride and isophthalic acid to give a copolymer. This partially unsaturated polymer undergoes further crosslinking to yield thermoset plastics. Related to this application, propylene glycol reacts with propylene oxide to give oligomers and polymers that are used to produce polyurethanes^[7] Propylene glycol is used as a humectant (E1520), solvent^[10] and preservative in food and for tobacco products. It is also one of the major ingredients (<1–92%), along with glycerol, of the e-liquid and cartridges used in electronic cigarettes where it is aerosolized in the atomizer.^[11] Propylene glycol is also used in various edible items such as coffee-based drinks, liquid sweeteners, ice cream, whipped dairy products and soda. [12][13] Vaporizers used for delivery of pharmaceuticals or personal-care products often include propylene glycol among the ingredients.^[7] Propylene glycol is used as a solvent in many pharmaceuticals, including oral, injectable and topical formulations, such as for diazepam and lorazepam which are insoluble in water. [14] Certain formulations of artificial tears, such as Systane, use proplyene glycol as an ingredien[15]

Like ethylene glycol, propylene glycol is able to lower the freezing point of water, and so it is used as aircraft de-icing fluid. [7][16] Water-propylene glycol mixtures dyed pink to indicate the mixture is relatively nontoxic are sold under the name of \underline{RV} or marine antifreeze. Propylene glycol is frequently used as a substitute for ethylene glycol in low toxicity, environmentally friendly automotive antifreeze. It is also used to winterize the plumbing systems in vacant structures. [17] The eutectic composition/temperature is 60:40 propylene glycol:water/-60 °C. The -50 °F/-45 °C commercial product is, however, water rich; a typical formulation is 40:60. [20]

Propylene glycol is used in veterinary medicine as an oral treatment for <a href="https://hyperketonaemia.com/hyperketonaemia.



Propylene glycol is often used in electronic cigarettes



A bottle of flavored 'e-liquid" for "vaping" shows propylene glycol as the main ingredient



Propylene glycol is commonly used to de-ice aircraft

Safety in humans

Oral administration

The acute oral toxicity of propylene glycol is very low, and large quantities are required to cause perceptible health damage in humans; propylene glycol is metabolized in the human body into <u>pyruvic acid</u> (a normal part of the glucose-metabolism process, readily converted to energy), <u>acetic acid</u> (handled by ethanol-metabolism), <u>lactic acid</u> (a normal acid generally abundant during digestion), [22] and <u>propionaldehyde</u> (a potentially hazardous substance). [23][24][25] According to the <u>Dow Chemical Company</u>, The LD50^[26] (Lethal Dose that kills in 50% of tests,) for rats is [27]20 g/mg (rat/oral).

Serious toxicity generally occurs at plasma concentrations over 4 g/L, which requires extremely high intake over a relatively short period of time, or when used as a vehicle for drugs or vitamins given intravenously or orally.^[28] It would be nearly impossible to reach toxic levels by consuming foods or supplements, which contain at most 1 g/kg of PG, except for alcoholic beverages in the US which are allowed 5 percent = 50g/kg.^[29] Cases of propylene glycol poisoning are usually related to either inappropriate intravenous administration or accidental ingestion of lage quantities by children.^[30]

The potential for long-term oral toxicity is also low. In one study, in 1972, 12 rats were provided with feed containing as much as 5% PG over a period of 2 years, and showed no apparent ill effects; no data on offspring were offered. Because of its low chronic oral toxicity, propylene glycol was classified by the U. S. Food and Drug Administration as "generally recognized as safe" (GRAS) for use as a direct food additive, including frozen foods such as ice cream and frozen desserts [29][32] The GRAS designation is specific to its use in food, and does not apply to other uses [33]

Skin, eye and inhalation contact

Prolonged contact with propylene glycol (E490) is essentially non-irritating to the skin.^[34] Undiluted propylene glycol is minimally irritating to the eye, producing slight transient <u>conjunctivitis</u>, the eye recovers after the exposure is removed. Exposure to mists may cause eye irritation, as well as <u>upper respiratory tract</u> irritation. Inhalation of propylene glycol vapors appears to present no significant hazard in ordinary applications.^[35] However, limited human experience indicates that inhalation of propylene glycol mists could be irritating to some individuals.^[36] It is therefore recommended that propylene glycol not be used in applications where inhalation exposure or human eye contact with the spray mists of these materials is likely, such as <u>simulated fogs</u> for theatrical productions, or antifreeze solutions for emegency eye wash stations.^[37]

According to a 2010 study by <u>Karlstad University</u>, the concentrations of PGEs (counted as the sum of propylene glycol and glycol ethers) in indoor air, particularly bedroom air, has been linked to increased risk of developing numerous respiratory and immune disorders in children, including <u>asthma</u>, <u>hay fever</u>, <u>eczema</u>, and allergies, with increased risk ranging from 50% to 180%. This concentration has been linked to use of water-based paints and water-based system cleansers. However, the study authors write that glycol ethers and not propylene glycol are the likely culprit. [38][39][40]

Propylene glycol does not causesensitization, and it shows no evidence of being a carcinogen or of beingenotoxic [41][42]

Intravenous administration

Adverse responses to <u>intravenous administration</u> of drugs that use propylene glycol as an <u>excipient</u> have been seen in a number of people, particularly with large dosages. Responses may include "hypotension, <u>bradycardia... QRS</u> and <u>T</u> abnormalities on the ECG, <u>arrhythmia</u>, cardiac arrest, serum <u>hyperosmolality</u>, <u>lactic acidosis</u>, and <u>haemolysis</u>". [43] A high percentage (12% to 42%) of directly-injected propylene glycol is eliminated or secreted in urine unaltered depending on dosage, with the remainder appearing in its <u>glucuronide</u>-form. The speed of <u>renal filtration</u> decreases as dosage increases, [44] which may be due to propylene glycol's mild anesthetic / <u>CNS-depressant</u> -properties as an alcohol. [45] In one case, intravenous administration of propylene glycol-suspended nitroglycerin to an elderly man may have induced coma andicidosis. [46]

Animals

Propylene glycol is an approved food additive for dog and sugar glider food under the category of animal feed and is generally recognized as safe for dogs, with an $\underline{LD_{50}}$ of 9 mL/kg. The $\underline{LD_{50}}$ is higher for most laboratory animals (20 mL/kg). However, it is prohibited for use in food for cats due to links the their body anemia.

Allergic reaction

Individuals who cannot tolerate propylene glycol experience inflamed dry skin in the facial area, or small red dots on the body. Investigators believe that the incidence of allergic contact dermatitis to propylene glycol may be greater than 2% in patients with eczema or fungal infections, which are very common in countries with lesser sun exposure, and lower than normal <u>vitamin D</u> balances. Therefore, propylene glycol allegy is more common in those countries.^[50]

Environmental

Propylene glycol is known to exert high levels of <u>biochemical oxygen demand</u> (BOD) during degradation in surface waters. This process can adversely affect aquatic life by consuming oxygen needed by aquatic organisms for survival. Large quantities of <u>dissolved oxygen</u>(DO) in the water column are consumed when microbial populations decompose propylene glyc⁶, 1:2-23

Sufficient dissolved oxygen levels in surface waters are critical for the survival of fish, macroinvertebrates, and other aquatic organisms. If oxygen concentrations drop below a minimum level, organisms emigrate, if able and possible, to areas with higher oxygen levels or eventually die. This effect can drastically reduce the amount of usable aquatic habitat. Reductions in DO levels can reduce or eliminate bottom feeder populations, create conditions that favor a change in a community's species profile, or alter critical food-web interactions. [51]:2–30

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External links

- Propylene glycolwebsite
- WebBook page for C3H8O2
- ATSDR Case Studies in Environmental Meitine: Ethylene Glycol and Propylene Glycol Toxicity U.S. Department of Health and Human Services(public domain)

- Propylene Glycol chemical product info: properties, production, applications.
- ChemSub Online: Propylene glycol

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