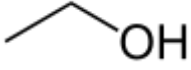

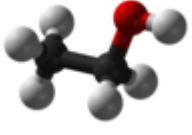




ETHANOL

	
$\begin{array}{c} \text{H} \quad \text{H} \\ \quad \\ \text{H}-\text{C}-\text{C}-\text{O}-\text{H} \\ \quad \\ \text{H} \quad \text{H} \end{array}$	
IUPAC name	Ethanol
Other names	Ethyl Alcohol; Grain Alcohol; Pure Alcohol; Hydroxyethane; Ethyl Hydrate
CAS	64-17-5
RTECS number	KQ6300000
SMILES	CCO
Molar Mass	46.06844(232) g/mol
Appearance	colorless clear liquid
Density	0.789 g/mL
Melting Point	-114.3 °C (158.8 K)
Boiling Point	78.4 °C, 173.1 F (351.6 K)
Solubility in Water	Fully miscible
Acidity (pKa)	15.9
Viscosity	1.200 mPa·s (cP) at 20.0 °C
Dipole Moment	5.64 fC·fm (1.69 D) (gas)
MSDS	External MSDS
EU classification	 F
NFPA 704	
R-phrases	R11 R20 R21 R22 R36
S-phrases	(S2), S7, S16
Flash Point	286.15 K (13 °C or 55.4 °F)
Except noted otherwise, materials data in their standard state at 25 °C, 100 kPa	

Ethanol, Ethyl Alcohol, Pure Alcohol is volatile, flammable colorless liquid. In common usage, it is often referred to simply as alcohol. Ethanol is abbreviated as EtOH, using common organic chemistry notation of representing the ethyl group (C₂H₅) with Et. Ethanol is a straight-chain alcohol, and its molecular formula is C₂H₅OH. An alternative notation is CH₃-CH₂-OH. Its empirical formula is C₂H₆O, making it a constitutional isomer of dimethyl ether. Except for use of fire, fermentation of sugar into ethanol is one of earliest organic reactions employed by humanity. Intoxicating effects of ethanol consumption have been known since ancient times. In modern times, ethanol for industrial use is also produced from by-products of petroleum refining. Ethanol has widespread use as a solvent of substances, including scents, flavorings, colorings, and medicines. In chemistry, is essential solvent and feedstock for the synthesis of other products. Long history as fuel for heat and light and also as fuel for combustion engines.

Ethanol is used by humans since prehistory. Dried residues on 9000-year-old pottery found in China imply that alcoholic beverages were used among Neolithic people. Its isolation as a relatively pure compound was first achieved by Persian alchemist Muhammad ibn Zakarīya Rāzi (Rhazes, 865–925). Geber (Jabir ibn Hayyan) and Al-Kindi (Alkindus) contributed to the development of distillation techniques. Writings attributed to Geber (721–815) mention flammable vapors of boiled wine. Al-Kindi (801–873) described the distillation of wine. In 1796, Johann Tobias Lowitz obtained pure ethanol by filtering distilled ethanol through activated charcoal. Lavoisier described ethanol as a compound of carbon, hydrogen, and oxygen. In 1808 Nicolas-Théodore de Saussure determined ethanol chemical formula. Fifty years later, Archibald Scott Couper published the structural formula of ethanol, which placed ethanol among first compounds whose chemical structure had been determined. Ethanol was first prepared synthetically in 1827 through the independent efforts of Henry Hennel in Great Britain and S.G. Sérullas in France. In 1828, Michael Faraday prepared ethanol by acid-catalyzed hydration of ethylene, a process similar to that which is used today for industrial ethanol synthesis.

Ethanol is a volatile, flammable, colorless liquid that has a strong characteristic odor. It burns with a smokeless blue flame that is not always visible in normal light. Physical properties of ethanol stem primarily from the presence of its hydroxyl group and the shortness of its carbon chain. Ethanol hydroxyl group is able to participate in hydrogen bonding, rendering it more viscous and less volatile than less polar organic compounds of similar molecular weight. Ethanol is a versatile solvent, miscible with water and with many organic solvents, including acetic acid, acetone, benzene, carbon tetrachloride, chloroform, diethyl ether, ethylene glycol, glycerol, nitromethane, pyridine, and toluene. It is also miscible with light aliphatic hydrocarbons, such as pentane and hexane, and with aliphatic chlorides such as trichloroethane and tetrachloroethylene. Ethanol's miscibility with water contrasts with that of longer-chain alcohols, whose

water miscibility decreases sharply as the number of carbons increases. Hydrogen bonding causes pure ethanol to be hygroscopic to the extent that it readily absorbs water from the air. The polar nature of the hydroxyl group causes ethanol to dissolve many ionic compounds, notably sodium and potassium hydroxides, magnesium chloride, calcium chloride, ammonium chloride, ammonium bromide, and sodium bromide. Sodium and potassium chlorides are slightly soluble in ethanol. Because ethanol molecule also has nonpolar end, it will dissolve nonpolar substances, including essential oils and numerous flavoring, coloring, and medicinal agents. Ethanol-water mixtures have less volume than the sum of their individual components.

Mixing equal volumes of ethanol and water results in only 1.92 volumes of mixture. The addition of even a few percent of ethanol to water sharply reduces the surface tension of water. This property partially explains the "tears of wine" phenomenon. Mixtures of ethanol and water (>50% ethanol) are flammable and easily ignited. Ethanol-water solutions that contain less than 50% ethanol may also be flammable if the solution is first heated. Ethanol is slightly more refractive than water, having a refractive index of 1.36242 (at $\lambda=589.3$ nm and 18.35 °C).

Chemical properties

Ethanol is classified as a primary alcohol, meaning that the carbon to which its hydroxyl group is attached has at least two hydrogen atoms attached to it as well. The chemistry of ethanol is largely that of its hydroxyl group.

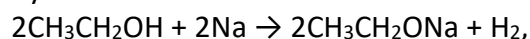
Acid-base chemistry

Ethanol's hydroxyl causes the molecule to be slightly basic.

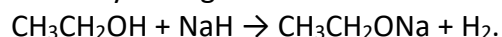
It is however, so very slightly basic it is almost neutral, like pure water.

The pH of 100% ethanol is 7.33, compared to 7.00 for pure water.

Ethanol can be quantitatively converted to conjugate base, ethoxide ion ($\text{CH}_3\text{CH}_2\text{O}^-$) by reaction with alkali metal such as sodium:



or a very strong base such as sodium hydride:



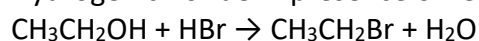
This reaction is not possible in an aqueous solution, as water is more acidic, so that hydroxide is preferred over ethoxide formation.

Halogenation

Ethanol reacts with hydrogen halides to produce ethyl halides such as ethyl chloride and ethyl bromide: $\text{CH}_3\text{CH}_2\text{OH} + \text{HCl} \rightarrow \text{CH}_3\text{CH}_2\text{Cl} + \text{H}_2\text{O}$

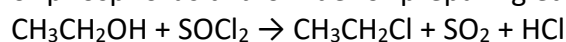
HCl reaction requires a catalyst such as zinc chloride.

Hydrogen chloride in presence of respective zinc chloride known as Lucas reagent.



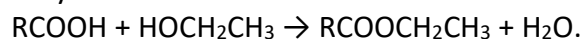
HBr requires refluxing with a sulfuric acid catalyst.

Ethyl halides can also be produced by reacting ethanol with more specialized halogenating agents, such as thionyl chloride for preparing ethyl chloride, or phosphorus tribromide for preparing ethyl bromide.



Ester formation

Under acid-catalyzed conditions, ethanol reacts with carboxylic acids to produce ethyl esters and water:



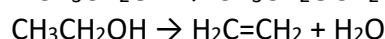
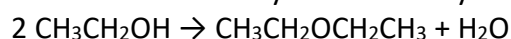
For this reaction it is necessary to remove water from the reaction mixture.

Ethanol can form esters with inorganic acids. Diethyl sulfate and triethyl phosphate, prepared by reacting ethanol with sulfuric and phosphoric acid respectively, are both useful ethylating agents in organic synthesis. Ethyl nitrite, prepared from the reaction

of ethanol with sodium nitrite and sulfuric acid, was formerly a widely-used diuretic.

Dehydration

Strong acid desiccants, such as sulfuric acid, cause ethanol's dehydration to form either diethyl ether or ethylene:



Diethyl ether or ethylene, predominates depends on precise reaction conditions

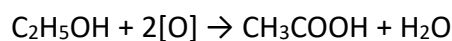
Oxidation

Ethanol can be oxidized to acetaldehyde, and further oxidized to acetic acid.

In the human body, these oxidation reactions are catalyzed by enzymes.

In laboratory, aqueous solutions of strong oxidizing agents, such as chromic acid or potassium permanganate, oxidize ethanol to acetic acid, and it is difficult to stop the reaction at acetaldehyde at high yield. Ethanol can be oxidized to acetaldehyde, without over oxidation to acetic acid, by reacting it with pyridinium chromic chloride.

The direct oxidation of ethanol to acetic acid using chromic acid is given below.



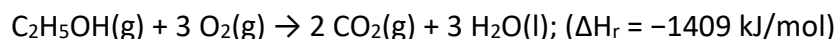
Oxidation product of ethanol, acetic acid, is spent as nutrient by the human body as acetyl CoA, where the acetyl group can be spent as energy or used for biosynthesis.

Chlorination

When exposed to chlorine, ethanol is both oxidized and its alpha carbon chlorinated to form the compound, chloral. $4\text{Cl}_2 + \text{C}_2\text{H}_5\text{OH} \rightarrow \text{CCl}_3\text{CHO} + 5\text{HCl}$

Combustion

Combustion of ethanol forms carbon dioxide and water:

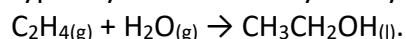


Production

Ethanol is produced both as a petrochemical, through the hydration of ethylene, and biologically, by fermenting sugars with yeast. Which process is more economical is dependent upon the prevailing prices of petroleum and of grain feed stocks.

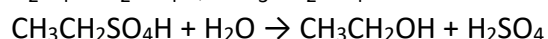
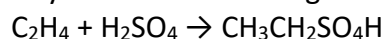
Ethylene hydration

Ethanol for use as industrial feedstock is often made from petrochemical feed stocks, typically the acid-catalyzed hydration of ethylene, represented by chemical equation



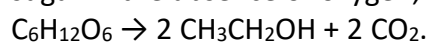
The catalyst is most commonly phosphoric acid, adsorbed onto a porous support such as diatomaceous earth or charcoal. This catalyst was first used for large-scale ethanol production by Shell Oil Company in 1947. The reaction is carried out with an excess of high pressure steam at 300°C.

In older process, first practiced on industrial scale in 1930 by Union Carbide, almost entirely obsolete, ethylene was hydrated indirectly by reacting it with concentrated sulfuric acid to produce ethyl sulfate, which was hydrolyzed to yield ethanol and regenerate the sulfuric acid:



Fermentation

When certain species of yeast (e.g., *Saccharomyces cerevisiae*) metabolize sugar in the absence of oxygen, they produce ethanol and carbon dioxide.



Culturing yeast under conditions to produce alcohol is called fermentation.

Cellulosic ethanol

Sugars for ethanol fermentation can be obtained from cellulose.

Deployment of this technology could turn number of cellulose-containing agricultural by-products into renewable energy resources.

Other enzyme companies are developing genetically engineered fungi that produce large volumes of cellulase, xylanase, and hemicellulase enzymes.

These would convert agricultural residues such as corn stover, wheat straw, sugar cane bagasse and energy crops into fermentable sugars.

Prospective technologies

Anaerobic bacterium *Clostridium ljungdahlii*, recently discovered in chicken wastes, can produce ethanol from single-carbon sources including synthesis gas, a mixture of carbon monoxide and hydrogen that can be generated from partial combustion of either fossil fuels or biomass. Use of bacteria to produce ethanol from synthesis gas has progressed to the pilot plant stage at Fayetteville, Arkansas USA.

Another prospective technology is closed-loop ethanol plant. Ethanol produced from corn has a number of critics who suggest that it is primarily just recycled fossil fuels because of the energy required to grow the grain and convert it into ethanol.

Though in early stage of research, there is some development of alternative production methods that use feed stocks such as municipal waste or recycled products, rice hulls, small diameter trees, wood chips, and switchgrass.

Purification

Ethylene hydration or brewing produces an ethanol–water mixture.

For most industrial and fuel uses, the ethanol must be purified.

Fractional distillation can concentrate ethanol to 95.6% by volume (89.5 mole%).

This azeotrope mixture with boiling point 78.1°C cannot be purified by distillation.

In one industrial method to obtain absolute alcohol, a small quantity of benzene is added to rectified spirit and the mixture is then distilled. Absolute alcohol is obtained in the third fraction, which distills over at 78.3°C. Because a small

amount of the benzene used remains in the solution, absolute alcohol produced by this method is not suitable for consumption, as benzene is carcinogenic. There is also an absolute alcohol production process by desiccation using glycerol. Alcohol produced by this method is known as spectroscopic alcohol—so called because the absence of benzene makes it suitable as a solvent in spectroscopy. Other methods for obtaining absolute ethanol include desiccation using adsorbents such as starch or zeolites, which adsorb water preferentially, as well as azeotropic distillation and extractive distillation.

Grades of ethanol

Denatured alcohol

Agents are added to ethanol to render it unfit to drink: bittering agents as denatonium benzoate, toxins such as methanol, naphtha, pyridine.

Products of this kind are called denatured alcohols.

Absolute ethanol

Absolute or anhydrous alcohol refers to purified ethanol, containing max 1% water. Absolute alcohol not intended for human consumption often contains trace amounts of toxic benzene (used to remove water by azeotropic distillation). Consumption of this form of ethanol can be fatal over a short time period. Generally this kind of ethanol is used as solvents for lab and industrial settings.

Use

Ethanol is easily miscible in water and is a good solvent.

Ethanol is less polar than water and is used in paints and tinctures.

Ethanol is also used in design and sketch art markers, such as Copic, and Tria.

2007-09-27 Source: Wikipedia