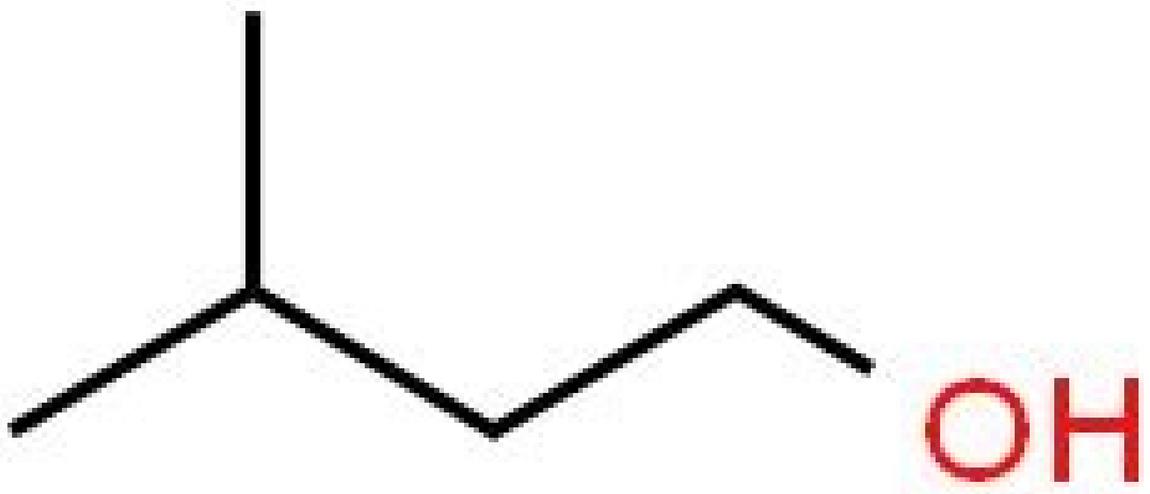
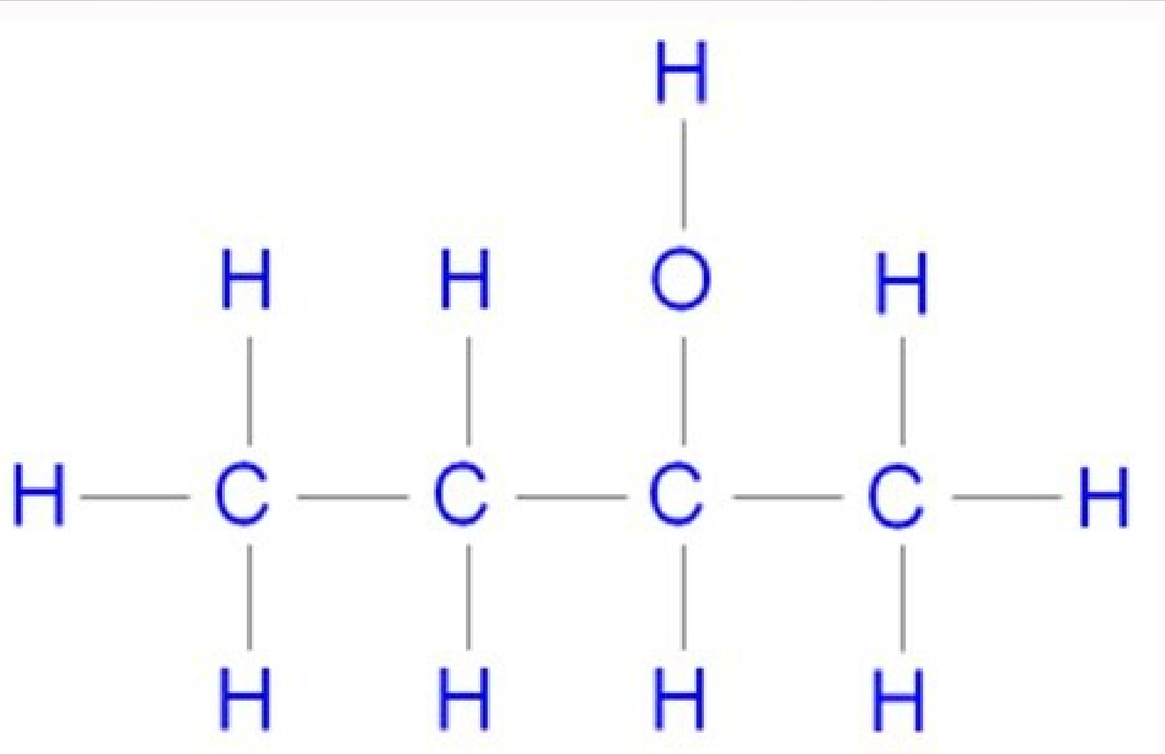
Butanol structural formula


OH


PRODUCT:
BUTANOL
TIANJIN SODA PLANT
E-MAIL: tjwmk@tjsoda.com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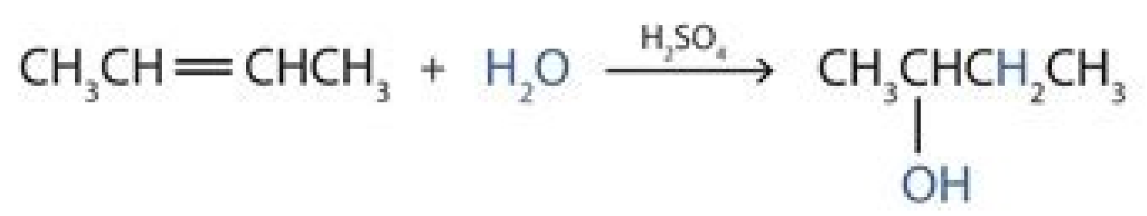

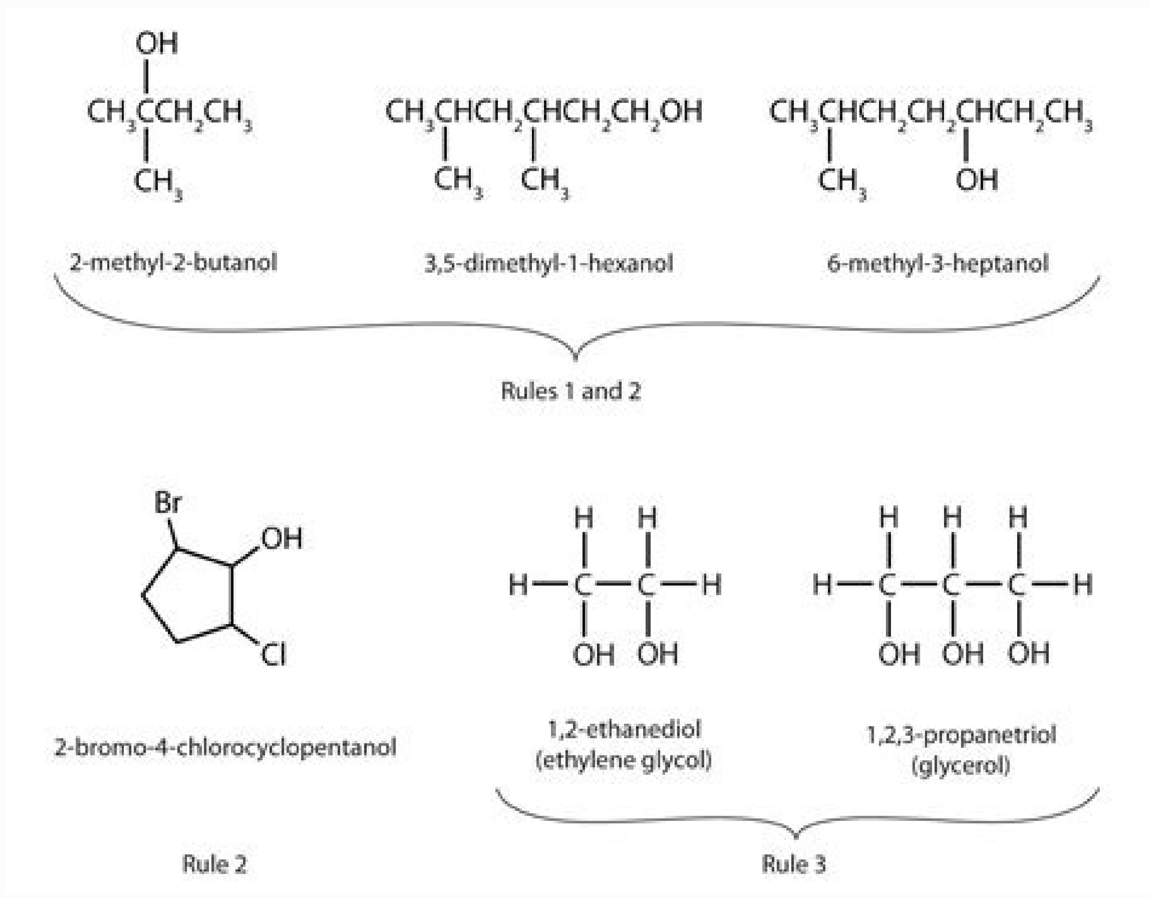

N-butanol structural formula. 3-methyl-2-butanol structural formula. 2-methyl-1-butanol structural formula. 3-butanol structural formula. 2-butanol structural formula. 3-methyl-1-butanol structural formula. 2-methyl-2-butanol structural formula. 1-butanol structural formula.

Chemical group Butanol (also called butyl alcohol) is a four-carbon alcohol with the formula C4H9OH found in five isomeric structures (four structural isomers), from a straight-chain primary alcohol to a branched-chain tertiary alcohol; [1], all of which are butyl or isobutyl attached to a hydroxyl group (sometimes referred to as BuOH, n-BuOH, i-BuOH and t-BuOH). It is n-butanol, 2 stereoisomers of sec-butanol, isobutanol and tert-butanol. Butanol is mainly used as a solvent and intermediate in chemical syntheses and can be used as a fuel. Biologically produced butanol is called biobutanol, which can be n-butanol or isobutanol. Isomers The unmodified term butanol usually refers to a straight-chain isomer with an alcohol function at the terminal carbon, also called n-butanol or 1-butanol. The straight-chain isomer with an alcohol on the inner carbon is sec-butanol or 2-butanol. The branched isomer with alcohol on the terminal carbon is isobutanol or 2-methyl-1-propanol and the branched isomer with alcohol on the inner carbon is tert-butanol or 2-methyl-2-propanol. n-butanol (1-butanol) sec-butanol (2-butanol) isobutanol (2-methylpropan-1-ol) tert-butanol (2-methylpropanol) Butanol isomers have different melting and boiling points. n-butanol and isobutanol have limited solubility, sec-butanol has much higher solubility while tert-butanol is miscible with water. The hydroxyl group makes the molecule polar, which promotes water solubility, while a longer hydrocarbon chain reduces polarity and solubility. Toxicity Butanol has a low level of toxicity in single dose experiments on laboratory animals [2] [3] and is considered safe enough for use in cosmetics. Brief, repeated overexposure to the skin may cause depression of the central nervous system, as with other short-chain alcohols. Exposure may also cause severe eye irritation and moderate skin irritation. Mainagainst prolonged exposure to alcohol vapors. In extreme cases, this includes central nervous system depression and even death. In most cases, butanol is rapidly metabolized to carbon dioxide. It has not been shown to damage DNA or cause cancer. Applications Main applications Butanol is used as a solvent in various chemical and textile processes, in organic synthesis and as a chemical intermediate. It is also used as a paint thinner and solvent in other coatings where a relatively slow evaporating latent solvent is preferred, such as in ambient temperature curing lacquers and enamels. It is also used as a component of hydraulic and brake fluids.[4] Since the 20th century, a 50% butanol solution in water has been used to slow down the drying of fresh plaster in fresco painting. The mortar is usually sprayed on the wet plaster after it has been leveled and smoothed, extending the working time in which the frescoes can be painted up to 18 hours. Butanol is used in the synthesis of 2-butoxyethanol. Butanol is primarily used as a reagent with acrylic acid in the production of butyl acrylate, the main component of water-based acrylic paints. It is also used as a perfume base, but has a strong alcohol aroma. Butanol salts are chemical intermediates; for example, the alkali metal salts of t-butanol are t-butoxides. Recreational use Butanol depresses the central nervous system. It can have ethanol-like effects when ingested or drunk by living beings such as humans. 85% butanol can be used in gasoline (petrol) vehicles without any engine modifications (unlike 85% ethanol) and contains more energy per volume than ethanol and almost as much as gasoline, and the use of butanol in a car will pay back the fuel consumption. , more comparable tolike ethanol. Butanol can also be added to diesel fuel to reduce soot emissions.[8] Photoautotrophic microorganisms such as cyanobacteria can be engineered to produce 1-butanol indirectly from CO2 and water.[9] Production Main article: Butanol fuel Since the 1950s, most butanol in the United States has been produced commercially from fossil fuels. The most common process starts with propene (propylene), which undergoes a hydroformylation reaction to form butanal, which is then reduced with hydrogen to 1-butanol and/or 2-butanol. tert-butanol is obtained from isobutane as a by-product in the production of propylene oxide. Butanol can also be produced by fermenting biomass with bacteria. Before the 1950s, Clostridium acetobutylicum was used in industrial fermentation to produce n-butanol. See also A.B.E. Process Fuel from Algae Butanol Fuel Solvent References Merck Index, 12th Edition, 1575 ^ Atsumi, S.; Hanai, T.; Liao, JC (2008). "Non-enzymatic routes to the synthesis of branched-chain higher alcohols as biofuels". Nature. 451 (7174): 86-9. doi:10.1038/nature06450. PMIDÂ 18172501. ^ 16 ECETOC JACC No. 41 n-butanol (CAS No. 71-36-3), European Center for Ecotoxicology and Chemical Toxicology, Brussels, December 2003, 3-4 p. ^ "n-butanol". Archived from the original on 2015-04-02. Retrieved 2012-02-03. ^ Isobutanol at chemicalland21.com ^ "Diego's Helpers | Diego Rivera Wall Project". www.riveramural.org. Downloaded on 27.03.2019. ^ Harris O.; and others. (August 1998). Toxicological profile of 2-butoxyethanol and 2-butoxyethanol acetate. US Department of Health and Human Services. ^ Sampa Maiti; and others. (December 10, 2015). "Searching for Sustainable Bioproduction and Recovery of Butanol as a Promising Fossil Fuel Solution". energy research. doi:10.1002/er.3458. ^ Antoni, D.; Zverlov, V. & Schwarz, W.H. (2007). "Biofuel from microbes". Applied microbiology and biotechnology. 77:23-35. doi:10.1007/s00253-007-1163-x. PMID 17891391. ^ Liu, X., Miao, R., Lindberg, P.,Lindblad, P. (2019). Modular engineering for efficient photosynthesis of 1-butanol biosynthesis from CO 2 in cyanobacteria. Energy & Environmental Science, 12(9), 2765-2777. Retrieved from " . page Secondary alcohol 2-butanol Names Preferred name IUPAC Butan-2-ol[2] Other names sec-butanol[1]]sec-butanol2-butanol2-butanol Identifiers CAS number 78-92-2Y14898-79-4 (R)Â Y4221-99-2 (S)Y 3D model (JSmol) Interactive image Beilstein Reference 4 (771647)) 1718763 (s) Chebi Chebi: 35687 y ChemBl ChemBl45462 y Chemspider 6320â Y76392 kar) â 25 drug (Y392 (R) u DB02606â Y ECHA Infocard 100.001.053 EC 201-158-5 GMELIN RESPONSE 16866. S) eye 2-butanol Pubchem CID 656884682â (r) 444683 (s) rtecs number 0203093 0203093 (2)5/h4-5H,3H2,1-2H3Â Key Y: BTANRVKWQNVYAZ-UHFFFAOYSA-NÂ Y SMILES CCC(C)O Properties Chemical formula C4H10O Molecular weight 74.123 g mol.8 cm. 3 Melting point -115°C; 175°F; 158 °K Boiling point 98-100 °C; 208 to 212°F; 371 to 373 K Water solubility 290 g/L[3] log P 0.683 Vapor pressure 1.67 kPa (at 20 °C) Acidity (pKa) 17.6 [4] Magnetic susceptibility (Ï) ≤718≤3•718 -3•5. 5 cm3 mola1 Refractive index (nD) 1.3978 (at 20 °C) Thermochemistry Heat capacity (C) 197.1 J Kâ1 molâ1 Std mol1 Std mol1 J 23 lmol 18 1 Std Enthalpy of formation (Îâ298â2.3â.1µ kJ molâ1 Standard Enthalpy of Combustion (ÎcHâ¦µ298) âcHâ¦µ298 â111 M. 1 GHS Hazard Label: Pictograms Signal Word Warning Standard Hazard Statements H226, H319, H335, H336 Precautionary Statements, P734eP2NF+101 1 3 0 Flash Point 22 ° C to 27 °C F; 295 to 300 K) Auto-ignition temperature 405 °C (761 °F; 678 K) Explosion limitsLethal Dose or Concentration (LD, LC): LCLo (lowest published) 16,000 ppm (rat, 4 hrs) 10,670 ppm (mouse, 3.75 hrs) 16,000 ppm (mouse, 2.67 hrs) [5] NIOSH (US health limits): PEL (Acceptable) TWA 150 ppm (450 mg/m3)[5] REL (recommended) TWA 100 ppm (305 mg/m3) ST 150 ppm (455 mg/m3)[5] IDLH (Immediate Hazard) 2000 ppm [5] Material Safety Data Sheet (SDS) inchem.org Related Compounds Butanols Related n-Butanol Isobutanoltert-Butanol Related Compounds Butanone Unless otherwise stated, data refer to materials in normal state (temperature 25°C [77°F], 100 kPa). Be sure to check (What is YN?) Information field References Chemical compound 2-butanol or sec-butanol is an organic compound with the formula CH3CH(OH)CH2CH3. Its structural isomers are 1-butanol. isobutanol and tert-butanol. 2-Butanol is chiral and can therefore be prepared as one of two stereoisomers, denoted (R)-(α)-2-butanol and (S)-(+)-2-butanol. It usually occurs as a 1:1 mixture of two stereoisomers - a racemic mixture. This secondary alcohol is a flammable, colorless liquid, soluble in three parts water and completely miscible with organic solvents. It is produced on a large scale, mainly as a precursor to the industrial solvent methyl ethyl ketone. (R)-(π)-2-butanol (S)-(+)-2-butanol Production and uses 2-butanol is produced industrially by the hydration of 1-butene or 2-butene: sulfuric acid is used as a catalyst. for this transformation.[6] In the laboratory, it can be made by the Grinard reaction of reacting ethylmagnesium bromide with acetaldehyde in dry diethyl ether or tetrahydrofuran. Although some 2-butanol is used as a solvent, it is mainly converted to butanone (methyl ethyl ketone, MEK), an important industrial solvent found in many household cleaners and paint removers. Though most paint removers have stopped using MEK in their products due to health issues and new regulations. Volatile 2-butanol esters have a pleasant taste and are usedamount in the form of fragrances or artificial flavors[6]. Solubility The reported solubility of 2-butanol is often incorrect [3], including some of the more familiar references such as the Merck Index, CRC Handbook of Chemistry and Physics, and Lange's Handbook of Chemistry. Even the International Program on Chemical Safety mentions incorrect solubility. This widespread error arose from Beilstein's "Handbuch der Organischen Chemie" ("Handbook of Organic Chemistry"). This paper gives a false solubility of 12.5 g/100 g water. Many other sources use this solubility, which has become a common mistake in the industrial world. The correct figures (35.0 g/100 g at 20 °C, 29 g/100 g at 25 °C and 22 g/100 g at 30 °C) were first published by Alekseev in 1886 by other scientists, including Dolgolenko and Dryer. in 1907 and 1913. Precautions Like other butanols, 2-butanol has low acute toxicity. LD50 is 4400 mg/kg (rat, oral).[6] Several explosions have been reported [7][8][9] during the normal distillation of 2-butanol, apparently due to a build-up of peroxides boiling higher than the pure alcohol (and thus the concentration in the still during distillation). Since it is generally known that alcohols, unlike ethers, are not capable of forming peroxide impurities, it is likely that the danger will be overlooked. 2-Butanol is a Class B peroxide-forming chemical. [10] Nomenclature of Organic Chemistry (IUPAC Blue Book), Sections A, B, C, D, E, F and H. Oxford: Pergamon Press. 1979. The designations isopropanol, sec-butanol, and tert-butanol are incorrect because there are no isopropane, sec-butane, and tert-butane hydrocarbons to which the suffix "-ol" can be added; these names should be avoided. However, isopropyl alcohol, sec-butyl alcohol, and tert-butyl alcohol are permitted (see Rule C-201.3) because isopropyl radicals,and tert-butyl exist ^ "2-Butanol - Compound Summary". PubChem compound. USA: National Center for Biotechnology Information. March 26, 2005. Identification and related records. Retrieved October 12, 2011. ^ ab Alger, Donald B. (November 1991). "Aqueous Solubility of 2-Butanol: A Common Mistake". 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MeSH 1-butanol PubChem CID number 263 RTECS EO1400000 UNII 8PJ61P6TS3 Y UN number 1120 CompTox Dashboard (EPA) DTXSID1021740 C4H1hI -UHFFFAOYSA-NÂ YInChi=1/C4H10O/c1-2-3-4-5/h5H,2-4H2 ,1H3 SMILES OCCCC Properties Chemical formula C4H10O Molecular weight 74.123 g molâkrâsa molainakrâsaòa¥1, Appearance -similar,[2] pungent, alcoholic and sweet Density 0.81 g/cm3 Melting point -89.8 °C (-129.6 ° 183.3 K) boiling point 117.7 °C (243.9 °C) °F; 390.8 K) water solubility 73 g/L at 25°C solubility very soluble in acetone miscible with ethanol, diethyl ether log P 0.839 vapor pressure 0.58 kPa (20°C) International Chemical Safety Data Sheets ILO ICSC) acidity (pKa) 16.10 Magnetic susceptibility (Ï) â56.536 10-6 cm3/mol Refractive index (nD) 1.3993 (20°C) Viscosity 2.573 mPa s (at]25 pol) Moment 1, 66 D Thermochemistry Standard molar entropy (Sâ¦ µ298) 225.7 J/ (K mol) h enthalpy of formation (ÎfHâ¦µ298) ≤328(4) kJ/mol h 0 Flash point 35 °C (95 °F; 308 ° K) Auto-ignition temperature 343 °C (649 °F; 616 K) Explosion limits 1.45-11.25% Lethal dose or concentration (LD, LC): LD50 (average dose) 790 mg/kg (raLot, mg/kg) (lowest published) 3484 mg/kg (rabbit, oral) 790 mg/kg (rat, oral) 1700 mg/kg (dog, oral)[5] LC50 (mean concentration) 9221 ppm (mammals) 8000 ppm (rats, 4 h)[5] N IOSH (US ves Occupational Exposure Limits): PEL (acceptable) TWA 100 ppm (3 00 mg/m3)[4] REL (recommended) C 50 ppm (150 mg/m3) [skin][4] IDLH (immediate hazard) 1400 ppm[4] Material Safety Data Sheet (SDS) ICSC 0111 Related compounds RelatedButanethiolbutylamine Diethyl etherPentane Unless otherwise stated, data refer to materials in their normal state (at 25 °C [77 °F], 100 kPa). N Check (what is YN?) Factbox Reference Chemical 1-butanol, also known as butan-1-ol or n-butanol, is a primary alcohol with the chemical formula C4H9OH and a linear structure. Isobutanol, butan-2-ol and tert-butanol are isomers of 1-butanol. The unmodified term butanol usually refers to the straight chain isomer. 1-Butanol occurs naturally as a byproduct of ethanol fermentation of sugars and other carbohydrates[6] and is found in many foods and beverages.[7][8] It is also an approved artificial flavoring agent in the United States [9] used in butter, cream, fruit, rum, whiskey, ice cream and ice cream, confectionery, baked goods, and spirits. It is also used in various consumer products.[7] The largest use of 1-butanol is as an industrial intermediate, especially for the production of butyl acetate (itself an artificial flavor and industrial solvent). It is a petrochemical product derived from propylene. Production estimates for 1997 are: US 784,000 tons; Western Europe 575,000 tonnes; Japan 225,000 tonnes. Production Since the 1950s, 1-butanol has been mainly produced by propene hydroformylation (oxo process), with n-butanal butyraldehyde being produced preferentially. Typical catalysts are based on cobalt and rhodium. The butyraldehyde is then hydrogenated to form butanol. The second way to produce butanol is the Reppe reaction of propylene with CO and water: [11] CH3CH=CH2 + H2O + 2 CO → CH3CH2CH2CH2OH + CO2 Previously, butanol was made from crotonaldehyde, which can be obtained from acetaldehyde. Butanol can also be produced by fermenting biomass with bacteria. Prior to 1950, Clostridium acetobutylicum was used in industrial fermentation to produce butanol. Research over the last few decades has shown what other microorganisms can dothrough fermentation. Industrial use 1-butanol, which accounts for 85% of its use, is mainly used in the production of varnishes. It is a popular solvent, i.e. for nitrocellulose. Various butyl ethers such as butoxyethanol are used as solvents. Many plasticizers are based on butyl ethers such as dibutyl phthalate. Butyl acrylate monomer is used to make polymers. It is a precursor of n-butylamines.[11] Biofuel 1-butanol has been proposed as a replacement for diesel and gasoline. It is produced in small quantities in almost all fermentations (see fusel oils). Clostridium provides a much higher yield of butanol. Research is underway to increase the production of biobutanol from biomass. Butanol is considered a potential biofuel (butanol fuel). 85% butanol can be used in gasoline-powered vehicles without any engine modifications (unlike 85% ethanol) and provides more power per volume than ethanol, almost the same as gasoline. Therefore, a vehicle using butanol will return a fuel economy more comparable to gasoline than to ethanol. Butanol can also be added to diesel fuel to reduce soot emissions.[12] Exposure to 1-butanol can be caused by the manufacture or in some cases the use of the following: artificial leather, butyl ether, rubber glue, dyes, fruit essences, varnishes, films and photographic films, raincoats, perfumes, pyroxylin plastic, viscose, safety glass, shellac and waterproof fabric. Natural Occurrence Butan-1-ol occurs naturally in the fermentation of carbohydrates in several alcoholic beverages, including beer,[13] grape brandy,[14] wine,[15] and whiskey.[16] It has been found in hops[17], jackfruit[18], boiled milk[19], eggplant,[20] cheese,[21] pea seeds[22] and cooked rice [. 23] 1-Butanol is also produced by frying corn oil, cottonseed oil, trilinolein and triolein.[24] Butan-1-ol is one of the "melting alcohols" (Nofor "poor spirits"), which include alcohols containing more than two carbon atoms and characterized by significant water solubility. It is a natural component of many alcoholic beverages, albeit in small and variable concentrations. It is believed (along with similar fusel alcohols) to cause a severe hangover, although experiments in animal models show no evidence of this. 1-Butanol is used as an ingredient in processed and artificial flavors[29] as well as in the extraction of lipid-free protein from egg yolks[30], natural flavors and vegetable oils, in the manufacture of hop extract for brewing, and as a solvent to remove pigments from wet concentrated protein from curd leaves.[31] metabolism and toxicity. The acute toxicity of 1-butanol is relatively low: oral LD50 values are 790–4360 mg/kg (in rats; comparable values for ethanol are 7000–15000 mg/kg) [8]. 32 [11] It is fully metabolized in vertebrates, as is ethanol: alcohol dehydrogenase converts 1-butanol to butyraldehyde; it is then converted to butyric acid by aldehyde dehydrogenase. Butyric acid can be completely metabolized to carbon dioxide and water via the β-oxidation pathway. In rats, only 0.03% of an oral dose of 2000 mg/kg was excreted in urine.[33] At sublethal doses, 1-butanol acts similarly to ethanol as a central nervous system depressant: a rat study found that the intoxicating effects of 1-butanol were about 6 times that of ethanol, possibly due to its slower conversion by alcohol dehydrogenase [34] Other Hazards Liquid Like most organic solvents, 1-butanol is a severe eye irritant; repeated skin contact can also cause irritation.[8] This is believed to be a general degreasing effect. No skin sensitization was observed. Irritation of the airways only occurs at very high concentrations (>2400 ppm) [35]. Butanol-1 has a flash point of 35°C.moderate fire hazard: slightly more flammable than kerosene or diesel, but less flammable than many other common organic solvents. Central nervous system depressant effects (similar to ethanol poisoning) are a potential hazard when handling 1-butanol indoors, although the odor threshold (0.2–30 ppm) is well below the concentration that would cause neurological effects.] See also Butanol Fuel External Links International Chemical Safety Data Sheet 0111 NIOSH Pocket Guide to Chemical Hazards. "#0076". National Institute for Occupational Safety and Health (NIOSH). Organization for Economic Co-operation and Development (OECD) SIDS Preliminary Assessment Report (OECD) IPCS Environmental Health Criterion 65: Butanols: Four Isomes IPCS Health and Safety Guide 3: 1-Butanol Reference^ "1-Butanol - Summary of Compounds" . PubChem project. USA: National Center for Information on Biotechnology. ^ [N-Butanol Product Information, The Dow Chemical Company, Form #327-00014-1001, p.1] ^ Dubey, Gyan (2008). 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Source: " Octanol names IUPAC preferred name Octane-1 -ol Other names 1-octanol; n-octanol; caprylyl alcohol; Oktylalkoholové identifikátory Číslo CAS 111-87-5Â Y 3D model (JSmol) Interaktivní obrázek Beilstein Reference 1697461 ChEBI CHEBI:16188 ChEMBL ChEMBL26215Â Y ChemSpider 932Â Y Číslo ECHA InfoCard 2937215 IHme Referenční číslo ECHA07 3178152 ECH208 EC 17172152 KEGG C00756 PubChem CID 957 UNII NV1779205DÂ Y CompTox Dashboard (EPA) DTXSID7021940 InChI InChI=1S/C8H18O/c1-2-3-4-5-6-7-8-9/hHBPy3H,KHFOy 2H,KHFO 2H -UHFFFAOYSA-N NinChI=1/C8H18O/c1- 2-3-4-5-6-7-8-9/h9H,2-8H2,1H3Key: KBPLFHHGFOOTCA-UHFFFAOYAH SMILES CCCCCCCCO Properties Chemical formula C8118 g molâ1 Appearance Colorless liquid[1] Odor Aromatic[1] Density 0 0, 83 g/cm3 (20°C)[1] Melting point 16°C (3°F; 257 K)[1] Boiling point 195°C (383°F; 468 K)[1] Water solubility 0.83 g/ cm3 (20 °C)[1] 3 g/L (20 °C)[1] Viscosity 7.36 cP[2] Danger GHS Signal Word: Pictograms Warning Standard Hazard Statements H319 Precautionary Statements P264, P280, P305+P351+P338, P337+P313 NFPA 704 (Fire Diamond) 1 2 0 The data listed applies to r Materials in standard condition (at 25 °C [77 °F], 100 kPa) unless otherwise noted. N check (what is YN?) Links to info box The chemical compound 1-octanol, also known as octan-1-ol, is an organic compound with the molecular formula CH3(CH2)7OH. It's a fatty alcohol. Many other isomers are also commonly known as octanols. is 1-octanolfor the synthesis of esters for use in perfumes and fragrances. It has a pungent smell. Octanol esters such as octyl acetate are found in essential oils.[3] It is used to evaluate the lipophilicity of pharmaceutical products. Octanol is obtained mainly in industry by oligomerization of ethylene using triethylaluminum, followed by oxidation of aluminum alkyl products. This pathway is known as the Ziegler alcohol synthesis [3]. An idealized synthesis is shown: Al(C2H5)3 + 9 C2H4 – Al(C8H17)3 Al(C8H17)3 + 3 O + 3 H2O – 3 HOC8H17 + Al(OH)3. alcohols that can be separated by distillation. The Kuraray process identifies an alternative 1-octanol pathway, but using a C4+C4 formation strategy. 1,3-butadiene dimerizes by adding one water molecule. This transformation is catalyzed by palladium complexes. The resulting doubly unsaturated alcohol is then hydrogenated. Water/octanol partition Main article: Octanol-water partition coefficient Octanol and water are immiscible. The partitioning of the compound between water and octanol is used to calculate the partition coefficient P of the molecule (often expressed as its logarithm to the base 10, log P). The water/octanol separation is a relatively good approximation of the separation of cytosol and lipid membranes in living systems.[5] Many skin absorption models assume that the stratum corneum/water partition coefficient is well approximated by a water/octanol partition coefficient function of the form ¡ (K w / o) {\displaystyle \log (K_{sc/w})= a +b \log (K_{w / o})} Where a and b are constants, K s c / w {\displaystyle K_{sc/w)) is the stratum corneum/water partition coefficient and K w/o { \displaystyle K_{w /o}} is the water/octanol partition coefficient. The values of a and b vary from document to document, but Cleek & Bunge [7] give values of a = 0, b = 0.74. SpecificationsUse With a flash point of 81°C, 1-octanol is flame retardant, although its autoignition temperature is only 245°C. 1-Octanol is mainly used as a precursor in perfumery.[3] It has been studied for the control of essential tremor and other types of involuntary neurological tremor, as evidence suggests that it can reduce tremor symptoms at lower doses than those required to achieve a similar level of symptomatic relief with ethanol, thereby reducing alcohol risk will . Alcohol intoxication therapeutic doses. dosage.[8] Hydrogen bonding of 1-octanol with Lewis bases. This is a Lewis acid in the ECW model and its acid parameters are EA=0.85 and CA=0.87. [9] See also references to 2-octanol ^ a b c d e f Institute for Occupational Safety GESTIS substance database entry ^ Bhattacharjee, A.; Roy, Minnesota (November 17, 2010). 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CID 20083 RTECS number RH0795000 UNII 66B0DD5E40 Y CompTox control panel (EPA) DTXSID0027014 InChI InChI=1S/C20H30N7O16P3/c21-9-2-1-3-216(011)(039-4-91)(03514-99) -19 5 -38-45(34.35)43-46(36.37)39-6-11-14(29)16(42-44(31.32)33) 20(41-11)27 -8- 25 -12-17(22)23-7-24-18(12)27/h1.3-4.7-8.10-11.13-16.19-20.28 -30X.2.5- 6 ,21H2,(H,34,35)(H,36,37)(H2,22,23,24)(H2,31,32,33) Key: IMPUPYZMUDSKSF-UHFFFAOYSA-NInChI=1/C20H30N7O16P3/c21- 9 -2-1-3-26(4-9)19-15(30)13(28)10(40-19)5-38-45(34.35) 43- 46(36.37)39- 6 -11-14(29)16(42-44(31.32)33)20(41-11)27-8-25-12-17(22)23-7-24-18(12)27/ h1,3-4,7-8,10-11, 13-16,19-20,28-30H,2,5-6,21H2,(H,34,35)(H,36,37)(H2 ,22,23,24) (H2,31,32, 33) Key: IMPUPYZMUDSKSF-UHFFFAOYAA SMILE CC(O)CCCCCC Properties Chemical formula C8H18O Molar mass 130.231 g mol1 Appearance Colorless liquid with characteristic odor[1] Density 0.820 7 (g/cm3) (20°C)[2] Melting point ≈ 38°C 36°F; 235 K)[6] Boiling point 178.5 °C (353.3 °F, 451.6 K)[6] Solubility in water 1.120 g/l[3] Log P 2.9[3] Vapor pressure 0.031 mbar (20 °C) 0.11 mbar (30 °C) 0.9 mbar (50 °C)[3] Henry's constant (kH) 1.23E-04 atm-m3/mol[3]Index (nD) 1.426 (20 °C)[4] Viscosity 6.2 cP[5] Thermochemistry Heat Capacity (C) 330.1 (J/mol*K) (298.5K)[1] Safety and health hazards in (Occupational health and safety / Safety): Eye hazard 2[3] Skin hazard 2[3] GHS labeling:[3] Pictograms Signal word Warning Hazard statement H226, H315, H319, H411, H412 Precautionary statements P210, P233, P240, P241, P242, P243 , P273 , P280, P303+P361+P353, P370+P378, P391, P403+P235, P501 Flash point 71°C (160°F; 344K)[3] K)[3] Explosion limit 0.8% vol. - 7.4% vol. [3] Dose or lethal concentration (LD, LC): LD50 (mean dose) >3.2 g/kg (rat, oral) 4 g/kg (mouse, oral)[7]. Unless otherwise noted, data is based on materials in the standard condition (at 25 °C [77 °F], 100 kPa). Links Infobox Chemical compound 2-octanol (octan-2-ol, 2-OH) is an organic compound with the molecular formula CH3CH(OH)(CH2)5CH3. It is a colorless oily liquid, slightly soluble in water but soluble in most organic solvents. 2-Octanol is one of the fatty alcohols. A secondary alcohol is chiral, although it is most commonly found as a racemic mixture. Production 2-Octanol is produced commercially by the decomposition of ricinoleic acid. The by-product is a mixture of sebacic acid ((CH2)8(CO2H)2). The main raw material is castor oil, which mainly consists of ricinoleic acid.[8] [9] Application 2-octanol is mainly used as: fragrance [7][10][11][12] low volatility solvent: various resins (paints and varnishes, adhesives, inks, etc.), agricultural chemicals, mining, etc... [13][14][15][16] Defoamers: Pulp and Paper Industry, Oil and Gas, Cement, Coatings, Coal, etc. Blowing Agents in Mineral Flotation[17] Wetting Agents Can also be used as a chemical intermediate in the manufacture of various other chemicals: Surfactants (Ethoxylates, Sulfates, Sulfate Esters, etc.) , cosmetic plasticizer esters (palmitate, adipate, maleate, stearate, myristate, etc.), [18] plasticizers (acrylates, maleates, etc.), pesticides: Dinocap [19] [20]Zinc dithiophosphate (ZDDP) Fragrance (salicylate) Used in the manufacture of perfumes and disinfectant soaps [21] Used to prevent foaming and as a solvent for fats and waxes [21] Used to study and control essential tremor and other types of involuntary tremor. neurological tremor [21] See also 1-Octanol Notes^a b "2-Octanol" at NIST/WebBook^ "Techniques de l'ingénieurÂ: Solvants organiques". Archived from the original on 2015-04-02. Retrieved 13.3.2015. ^ a b c d e f g h i j Entry for 2-octanol in the Occupational Safety and Health Institute's GESTIS substance database, retrieved February 2, 2010, chemiabook.com. Archived from the original on 2015-04-02. Retrieved 10.05.2019. ^ Handbook of Industrial Solvents, Revised and Expanded by Nicholas P. Cheremisinov - p.7. ^ a b "2-Octanol" at ChemIDplus ^ a b "Alcool caprylique secondaire". csst.qc.ca (in French). Archived from the original on 2015-04-02. Retrieved 10.05.2019. ^ Cornil, boy; Lappen, Peter (2014). "Aliphatic dicarboxylic acids". Ullmann's Encyclopedia of Industrial Chemistry. Weinheim: Wiley-VCH. doi:10.1002/14356007.a08_523.pub3. ^ "Example of industrial use of castor oil derivatives". OCL Journal. Archived from the original on 2015-09-24. Retrieved 10.05.2019. ^ "2-octanol, 123-96-6". thegoodscentscompany.com. Archived from the original on 2006-06-05. Retrieved 10.05.2019. ^ Handbook of Fenarol Flavor Ingredients, 5th Edition George A. 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Links Synthetic/2-octano Source: 1084769175"Page 6 2-Heptanol[1] Names IUPAC Preferred Name Heptan-2-ol Other Names s-Heptyl Alcohol Identifiers CAS Number 543-49-7Â Y 3D Model (JSmol) Interactive Image ChEBI CHEBI BLUE 4 ChEM215Chm2014Chm2858 Y ECHA Information card 100.008.041 PubChem CID 10976 UNII E12FIG07JK Y CompTox control panel (EPA) DTXSID1047158 InChI InChI=1S/C7H16O/c1-3-4-5-6-h-7(2H) -2H3 YKey: CETWDUZRCINIHU-UHFFFAOYSA-NYInChI= 1 /C7H16O/c1-3-4-5-6-7(2)8/h7-8H,3-6H2,1-2H3 Key: CETWDUZRCINIHU-UHFFAOYAL SMILES OC (C) CCCCC properties Chemical formula C7H16O Molecular weight 116.201 g / mol Density 0.817 g/ml Melting point ≤30.2°C (Δ22.4°F; 243.0°K) Boiling point 159°C (318°F solubility 2°K) in water; 3.3 g/ l Solubility in ethanol, diethyl ether Viscosity 3.955 mPa s Dangerous temperature flash range 71°C (160°C; 344 K) Unless otherwise stated, data refer to materials under normal conditions (at 25°C100kPa). YÂ werifyÂ (what is YNÂ?) Infobox Links Chemical compound 2-Heptanol is a chemical compound that is an isomer of heptanol. It is a secondary alcohol with a hydroxyl group on the second carbon of a seven carbon straight chain. 2-Heptanol is chiral, so there are (R) and (S) isomers. See also 1-Heptanol 3-Heptanol 4-Heptanol Reference ^ Lide, David R. (1998), Handbook of Chemistry and Physics (87, ed.), Boca Raton, FL: CRC Press, pp. 3–300, 6– 189, 8–109, 16â25, ISBN 0-8493-0594-2 This alcohol article is a stub. You can help Wikipedia by expanding it. Other Names Heptyl Alcohol – Heptyl Alcohol Enanthyl Alcohol Identifiers CAS Number 111-70-6 Y 3D Model (JSmol) Interactive Image ChEBI CHEBI:43003 ChEMBL ChEMBL273459 Y ChemSpider 7837 Y ECHA5508 CCHASH 408 Comp. DTXSID8021937 InChI InChI=1S/C7H16O/c1-2-3-4-5-6-7-8/h8H,2-7H2,1H3YKey:BBMCTIGTTCKYKF-UHFFFAOYSA-N3YInH16O/1/C7InH16O -4-5-6 -7- 8/h8H,2-7H2,1H3Key: BBMCTIGTTCKYKF-UHFFFAOYAV SMILES OCCCCCCC Properties Chemical Formula C7H16O Molecular Weight 116.204 g molâ1 Density 7 g/346 cm1 Density 0.381 cm °C (≤30.3°F; 238.6 K) Boiling Point 175, 8 °C (348.4 °F; 448.9 °K) Magnetic Susceptibility (Ï) -91.7 cm3/mol Refractive Index (nD) 1.423 Thermochemistry Standard Enthalpy of Combustion (ÎcHâ¦µ298) - 4637.9 kJ/mol Hazards NFPA 704 (Fire Diamond) 2 2 0 Flash Point 76 °C (169 °F; 349 K) Data refers to materials in the normal state (at 25 °C [77 °F]], 100 kPa). YÂverify (what is YNÂ?) Links to info box The chemical compound 1-heptanol is a seven-carbon chain alcohol with the structural formula CH3(CH2)6OH.[1] It is a clear, colorless liquid that is very slightly soluble in water, but miscible with itand ethanol. Overview There are three other straight-chain isomers of heptanol, 2-heptanol, 3-heptanol and 4-heptanol, which differ in the position of the alcohol functional group. Heptanol is commonly used in cardiac electrophysiology experiments to block gap junctions and increase axial resistance between myocytes. An increase in axial resistance decreases conduction velocity and increases the heart's susceptibility to repetitive firing and sustained arrhythmias. 1-Heptanol has a pleasant smell and is used in cosmetics because of its smell. See also 2-Heptanol 3-Heptanol References ^ CRC Handbook of Chemistry and Physics (65th Edition). Retrieved from " Page 8 Names of 3-Heptanol IUPAC Preferred Name Heptan-3-ol Identifiers CAS Number 589-82 -2Â N 3D Model (JSmol) ChEMBL Interactive Image ChEMBL452729 Y ChemSpider 11036 Y ECHA Information Card 100 008 784 PubChem CID 11520 UNII 12YBT48HMK Y CompTox Dashboard -2HKQ16-HSA2Y,2/2/6HK7SA2Y)CCCC Properties Chemical Formula C7H16O Molar Mass, except Cases 20 4, mol , where g mol is given for materials in their standard state (at 25 °C [77 °F], 100 kPa). Do not check (What is YN?) Links to information fields The chemical compound 3-heptanol or heptan-3-ol is an organic alcohol with the chemical formula C7H16O.[1] 3-Heptanol is chiral, so there are (R) and (S) isomers. References ^ 3-Heptanol, ChemSpider See also 1-Heptanol 2-Heptanol 4-Heptanol This alcohol article is incomplete. You can help Wikipedia by expanding it. .php?title=3-Heptanol&oldid=1064281974"