Preparation of benzoic acid from benzamide pdf

Chemical compound Benzoic acid Names Preferred IUPAC name Benzoic acid[1] Systematic IUPAC name Benzenecarboxylic acid Other names CarboxybenzeneE210Dracylic acidPhenylmethanoic acidBzOH Identifiers CAS Number 65-85-0 Y 3D model (JSmol) Interactive image 3DMet B00053 Beilstein Reference 636131 ChEBI CHEBI:30746 Y ChEMBL ChEMBL541 Y ChemSpider 238 Y DrugBank DB03793 Y ECHA InfoCard 100.000.562 EC Number 200-618-2 E number E210 (preservatives) Gmelin Reference 2946 KEGG D00038 Y MeSH benzoic+acid PubChem CID 243 RTECS number DG0875000 UNII 8SKN0B0MIM Y CompTox Dashboard (EPA) DTXSID6020143 InChI InChI=1S/C7H6O2/c8-7(9)6-4-2-1-3-5-6/h1-5H,(H,8,9) YKey: WPYMKLBDIGXBTP-UHFFFAOYSA-N YInChI=1/C7H6O2/c8-7(9)6-4-2-1-3-5-6/h1-5H,(H,8,9)Key: WPYMKLBDIGXBTP-UHFFFAOYAD SMILES O=C(O)c1ccccc1 Properties Chemical formula C7H6O2 Molar mass 122.123 g·mol−1 Appearance Colorless crystalline solid Odor Faint , pleasant odor Density 1.2659 g/cm3 (15 °C) 1.0749 g/cm3 (130 °C)[2] Melting point 122 °C (252 °F; 395 K)[7] Boiling point 250 °C (482 °F; 523 K)[7] Solubility in water 1.7 g/L (0 °C) 2.7 g/L (18 °C) 3.44 g/L (25 °C) 5.51 g/L (40 °C) 21.45 g/L (75 °C) 56.31 g/L (100 °C)[2][3] Solubility soluble in acetone, benzene, CCl4, CHCl3, alcohol, ethyl ether, hexane, phenyls, liquid ammonia, acetates Solubility in methanol 30 g/100 g (-18 °C) 32.1 g/100 g (-13 °C) 71.5 g/100 g (23 °C)[2] Solubility in ethanol 25.4 g/100 g (-18 °C) 47.1 g/100 g (15 °C) 52.4 g/100 g (19.2 °C) 55.9 g/100 g (23 °C)[2] Solubility in acetone 54.2 g/100 g (20 °C)[2] Solubility in olive oil 4.22 g/100 g (25 °C)[2] Solubility in 1,4-Dioxane 55.3 g/100 g (25 градусов по Цельсию) журнал P 1.87 Давление пара 0.16 Pa (25 C) 0.19 kPa (100 C) 22.6 kPa (100 c) 22.6 kPa (200 c) Кислотность (pKa) 4.202 (H2O χ) 1,5397 (20 градусов по Цельсию) 1,50 см3/мол рефракционный индекс (nD) 1,5397 (20 градусов по Цельсию) 1,504 (132 C) 1.26 mPa (130 C) Структура Кристаллическая структура Моноклиническая Молекулярная форма планарный диполь момент 1.72 D в диоксане Термохимия Тепловая емкость (C) 146.7 J/mol K.4. Стид Моларентропия (So298) 167,6 J/mol K[2] Std enthalpy offormation (ΔfH⊖298) -385.2 kJ/mol[2] Std enthalpy ofcombustion (ΔcH⊖298) -3228 kJ/mol[4] Hazards Main hazards Irritant Safety data sheet JT Baker GHS pictograms [8] GHS Signal word Danger GHS hazard statements H318, H335[8] GHS precautionary statements P261, P280, P305+351+338[8] NFPA 704 (fire diamond) 1 2 0 Flash point 121.5 °C (250.7 °F; 394.6 K)[7] Autoignitiontemperature 571 °C (1,060 °F; 844 K)[7] Lethal dose or concentration (LD, LC): LD50 (median dose) 1700 mg/kg (rat, oral) Related compounds Related carboxylic acids Hydroxybenzoic acidsAminobenzoic acids,Nitrobenzoic acids,Phenylacetic acid Related compounds Benzaldehyde,Benzyl alcohol,Benzoyl chloride,Benzylamine,Benzamide Except where otherwise noted, data for materials in their standard condition (at 25 degrees Celsius, 100 kPa). Y check (what is yn?) Infobox refers to benzoic acid /bɛnˈzoʊ.ɪk/ is white (or colorless) solid with the C6H5CO2H formula. It is the simplest aromatic carboxicycil acid. The name comes from benzoin gums, which for a long time was its only source. Benzoic acid occurs naturally in many plants and serves as an intermediate in the biosynthesis of many secondary metabolites. Benzoic acid salts are used as food preservatives. Benzoic acid is an important precursor to the industrial synthesis of many other organic substances. The salts and esters of benzoic acid are known as benzoates /ˈbɛnzoʊ.eɪt/. The history of benzoic acid was discovered in the sixteenth century. Dry distillation of benzoin gums was first described by Nostradamus (1556) and then by Alexius Pedemontanus (1560) and Blaise de Vigener (1596). The composition of benzoic acid was determined by Hustus von Liebig and Friedrich Wehler. These latter have also investigated how hipporic acid is associated with benzoic acid. In 1875, Salkovsky discovered the antifungal abilities of benzoic acid, which has long been used to preserve the benzo-containing fruit of berries. It is also one of the chemical compounds found in the castor. This compound is collected from castor bags of North American beaver. The production of industrial preparations of benzoic acid is made on a commercial basis by partial oxygen oxygen oxidation of toluene. The process is catalyzed with cobalt or manganese moths. The process uses abundant materials, and continues in high yields. The first industrial process is associated with the reaction of benzothyrchloride (trichloromethylbenzene) with calcium hydroxide in water, using iron or iron salt as a catalyst. The resulting calcium benzoate is converted into benzoic acid with salt acid. The product contains a significant amount of derivatives of chlorinated benzoic acid. For this reason, benzoic acid for human consumption was obtained by dry distillation of benzoin gums. Food benzoic acid is currently produced synthetically. Laboratory synthesis of benzoic acid is cheap and readily available, so laboratory synthesis of benzoic acid is mainly practiced for its pedagogical value. This is the usual training of students. The benzoic acid can be cleaned by redistricting from the water due to its high salt in hot water and bad solubility in cold water. Avoiding organic solvents for re-crystalization makes this experiment particularly safe. This process usually yields output of about 65% (14) on hydrolysis As well as other nitriles and amide, benzonitril and benzamid can be hydrolysed with benzoic acid or its conjugation base in acidic or basic conditions. Of bromoben can be converted into benzoic acid by carboxylation of the intermediate intermediate Bromide. This synthesis offers a convenient exercise for students to perform Grignard's reaction, an important class of carbon-carbon bonds that form reactions in organic chemistry. The oxidation of benzyl compounds of benzyl alcohol and benzylchloride and virtually all benzil chloride derivatives is easily oxidized to benzoic acid. The use of benzoic acid is mainly consumed in the production of phenol by oxidative decarboxilation at 300-400 degrees Celsius: 23 x 5HCO2H, 1/2 O2 → C6H5OH and CO2 Required temperature can be reduced to 200 degrees Celsius by adding cot decals (II) salts. Phenol can be converted into cycloxexanol, which is the starting material for the synthesis of nylon. Precursors of plasticizers of benzoate plasticizers, such as glycol-, diethylene glycol and triethylene glycol estuaries, are obtained by transesterification of methyl benzoate corresponding diol. As an alternative, these species occur in the treatment of benzoyl chloride diol. These plasticizers are used in the same way as those derived from the teretalic acid ester. The precursor to sodium benzoate and associated preservatives benzoic acid and its salts is used as food preservatives represented by E numbers E210, E211, E212 and E213. Benzoic acid inhibits the growth of mold, yeast and some bacteria. It is either added directly or created from reactions with its sodium, potassium or calcium salt. The mechanism begins with the absorption of benzoic acid into the cell. If the intracellular pH changes by 5 or below, the anaerobic fermentation of glucose through phosphofructokinase is reduced by 95%. The effectiveness of benzoic acid and benzoate thus depends on the pH of the food. Acid and beverages such as fruit juice (lemon acid), sparkling drinks (carbon dioxide), soft drinks (phosphoric acid), pickles (vinegar) or other acidic foods are stored with benzoic acid and benzoate. Typical levels of using benzoic acid as a preservative in food are between 0.05-0.1%. Foods in which benzoic acid can be used and maximum levels for its use are controlled by local food laws. Concerns were expressed that benzoic acid and its salts could react with ascorbic acid (vitamin C) in some soft drinks, forming a small amount of carcinogenic benzene. Cm. also: Benzene in soft drinks Medicinal benzoic acid is an integral part of Whitfield's ointment, which is used to treat fungal skin diseases such as shingles, ringworm, and athlete's feet. As the main component of benzoin gums, benzoic acid is also the main ingredient in both benzoin tinctures and Monk. Such products have a long history of use as topical antiseptics and inhalation decongestants. Benzoic acid was used as a waiter, analgesic and antiseptic in the early 20th century. Benzoyl chloride benzoic acid is a precursor to benzoyl benzoyl C6H5C (O)Cl by treating thionylchloride, phosgene or one of phosphorus chlorides. Benzoyl chloride is an important starting material for several benzoic acid derivatives, such as benzyl benzoate, which is used in artificial flavors and insect repellents. Niche and laboratory use In training laboratories benzoic acid is a common standard for calibrating the calibration of the bomb's calibration. Biology and the health effects of benzoic acid occur naturally, as do its esters in many species of plants and animals. A palpable amount is found in most berries (about 0.05%). Ripe fruits of several types of vaccine (e.g. cranberries, macrocarpone V. vitis; blueberries, V. myrtillus) contain up to 0.03-0.13% free benzoic acid. Among animals, benzoic acid has been found mainly in omnivorous or phytophagic species, such as in the innards and muscles of the Ptarmigan rock (Lagopus muta), as well as in the secretions of male musk glands (Ovibos moschatus) or Asian bull elephants (Elephas maximus). benzoic acid and 40% of the esters of benzoic acid. In terms of biosynthesis, benzoate is produced in plants from cytnamic acid. The pathway was determined from phenol using 4-hydroxybenzoate. Reactions of benzoic acid can occur either in the fragrant ring or in the carboxyl group: Aromatic ring electrophilic aromatic replacement reaction will occur mainly in 3-positional due to the electronically-washed carboxic imaging group; i.e. benzoic acid is a meta-direction. Carboxyl Group Reactions typical of carboxyl acids are also applied to benzoic acid. Benzoate esters are a product of acid catalytic reaction with alcohol. Amide benzoic acid is usually made from benzoyl chloride. Dehydration of benzoic anhydride is induced by acetic anhydride or phosphorus pentoxide. Highly reactive derivative acids, such as acid halides, are easily produced by mixing with halogening agents such as phosphorus chlorides or thionilchloride. Orthopedists can be obtained as a result of alcohol reaction in conditions free of acidic water with benzonitril. Reducing benzaldehyde and benzyl alcohol is possible with DIBAL-H, LiAlH4 or sodium borohydride. Decarboxiling benzene can be caused by heating in the cinema in the presence of copper salts. Hunsdiecker decarboxylation can be achieved by heating silver salt. The safety and metabolism of mammals It stands out as hypuric acid. Benzoic acid is metabolized by butyrat-coA ligase in an intermediate product, benzoyl-CoA, which is then metabolized by Glycine N-aciltranspheras in hypuric acid. People metabolize toluene and benzoic acid, which is secreted as Acid. For people, the World Health Organization's International Programme on Chemical Safety (IPCS) offers Tolerant consumption will be 5 mg/kg of body weight per day. Cats have a significantly lower tolerance to benzoic acid and its salts than rats and mice. The lethal dose for cats can be as low as 300 mg/kg of body weight. Oral LD50 for rats is 3040 mg/kg, for mice it is 1940-2263 mg/kg. 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International Chemical Safety Map 0103 SIDS Initial Benzoic Acid Assessment Report from the Organisation for Economic Co-operation and Development (OECD) ChemicalLand Obtained from 2 4-Aminobenzoic Acid Names Preferred IUPAC Name 4-Aminobenzoic Acid Other Names Para-aminobenzoic Acid-Aminobenzoic AcidPABAVitamin B10Vitamin BxBacterial Vitamin H1 ID CAS Number 1 1 ChEBI CHEBI:30753 Y ChEMBL ChEMBL542 Y ChemSpider 953 Y DrugBank DB02362 Y ECHA Info Map 100.005.231 KEGG D02456 Y PubChem CID 978 UNII TL2TJE8'tX Y CompTox Dashboard (EPA) DTXSID6024466 InChi SMILES O'C(O)c1ccc (N)cc1 Properties Chemical Formula C7H7NO2 Molar mass 137,138 gm mole-1 Appearance white-gray crystals Density 1,374 g/ml melting point 187 to 189 degrees Celsius (369 to 372 F; 460 to 462 k) Boiling point 340 degrees Celsius (644 degrees Fahrenheit; 613 k) Can be used in water 1 g/170 ml (25 degrees Celsius) 1 g/90 ml (90 degrees Celsius) Acidity (pKa) 2.50 (carboxil; H2O)4.87 (ameno; H2O) Dangers of a major eye hazard irritant, some people may be allergic to this compound Except when otherwise noted, the data are given for materials in their standard condition (at 25 degrees Celsius, 100 kPa). Y check (what is yn?) Infobox links 4-aminobenzoic acid (also known as para-aminoomasoneic acid or PABA because the number 4 carbon in the benzene ring is also known as steam position) is an organic compound with the H2NC6H4CO2H formula. PABA is white solid, although commercial samples may appear gray. It's a little soluble in the water. It consists of a benzene ring, replaced by amino acids and carboxyl groups. The connection occurs widely in the natural world. Manufacturing and Emergence In industry, PABA is prepared mainly by two routes: Reducing hoffman's 4-nitrobenzoic acid degradation of monoamide derived from terephthic acid. PABA's food sources include liver, beer yeast (and unfiltered beer), kidneys, molasses, mushrooms and whole grains. Overview of this connection. Biology Biochemistry Tetrahydrofolate synthesis pathway PABA is intermediate in the synthesis of folic acid bacteria, plants and fungi. Many bacteria, including those found in the human gastrointestinal tract, such as E. coli, generate PABA from chorismate as a result of the combined action of enzymes 4-amino-4-disihorismate and 4-amino-4-deichorism lyase. Plants produce PABA in their chloroplasts and store it as a glucose ester (pABA-Glc) in their tissues. People lack enzymes to convert PABA into folate, so they require folic acid from dietary sources such as green leafy vegetables. In humans, PABA is considered inconsequential and although it has been named historically as vitamin Bx, is no longer recognized as a vitamin because most people (citation is necessary) have a microbiome that will generate PABA. Sulfonamid drugs are structurally similar to PABA, and their antibacterial activity is due to their ability to interfere with the conversion of PABA into folate by the enzyme dihydropteroate synthetas. Thus, bacterial growth is limited due to folic acid deficiency. The medical use of potassium salt is used as a drug against fibrous skin diseases such as Peyronie's disease, under the trade name Potaba. PABA is also used from time to time as a irritable bowel syndrome sufferers to treat related gastrointestinal symptoms, as well as in food epidemiological studies to assess the completeness of a 24-hour urine collection to determine the urinary sodium, potassium or or or Levels. Nutritional supplement Despite the absence of any recognized PABA deficiency syndromes in humans, except for those who lack the intestinal bacteria that generate PABA, many claims benefit made by commercial PABA suppliers as a dietary supplement. The benefits are claimed for fatigue, irritability, depression, crying eczema (wet eczema), scleroderma (premature hardening of the skin), spotted loss of pigment in the skin (vitiligo), and premature gray hair. Commercial and industrial use of PABA is used mainly in the biomedical sector. Other uses include its conversion to specialty azo dyes and cross agents. PABA is also used as a biodegradable pesticide, although its use is currently limited due to the evolution of new bio-pesticide variants. In the past, PABA has been widely used in sunscreens as a UV filter. It is a UVB shock absorber, which means it can absorb wavelengths between 290 and 320 nm. Patented in 1943, PABA was one of the first active ingredients to be used in sunscreens. The first in vivo studies on mice have shown that PABA has reduced UV damage. It has also been shown to protect against skin tumors in rodents. Animal and in vitro studies in the early 1980s have shown that PABA can increase the risk of uvim cell damage. Based on these studies, as well as problems with allergy and discoloration of clothing, PABA fell out of place like sunscreen. However, water-soluble PABA derivatives such as padimate O are currently used in some products. PABA's safety considerations are largely non-toxic; The average lethal dose of PABA in dogs (oral) is 2 g/kg. It is formed in the metabolism of some esther local anesthesia, and many allergic reactions to local anesthetics are the result of reactions to PABA. Cm. also 4-Ainosalicylic Acid Links - Haynes, William M., Ed. (2016). CRC Press. 5-89. ISBN 978-1498754286. B Mackie, T.; Takeda, K. (2000). Benzoic acid and derivatives. Encyclopedia of Ullman's Industrial Chemistry. Wiley-HF. doi:10.1002/14356007.a03_555. Food resource for health. Archive from the original 2009-12-16. Received 2009-11-21. Key, Alisha; Popek, Tomas; Kiyota, Tyra; de Macedo, Pierre; Stefanovic, Peter; Carmen Lazar; Konishi, Yasuo (2002). The evolution of drugs: p-aminobenzoic acid as a building block. Current medicinal chemistry. 9 (21): 1871–1892. doi:10.2174/0929867023368872. ISSN 0929-8673. b Para-aminebenzoic acid. Medline Plus Medical Encyclopedia. National Institutes of Health of the United States. 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