

☐

I'm not robot


reCAPTCHA

I am not robot!

What is the chemical formula of butanedioic acid

What is the chemical formula of butanoic acid. **What is the formula for butanoic acid.** **What is butanoic acid.** **Which of the following is the formula of butanoic acid.** **What is the structural formula for butanoic acid.**

Please enable Javascript in order to use PubChem website. Chemical compound Butyric acid Skeletal structure of butyric acid Flat structure of butyric acid Names Preferred IUPAC name Butanoic acid[1] Other names Ethylacetic acid1-Propanecarboxylic acidPropylformic acidC4:0 (Lipid numbers) Identifiers CAS Number Butyric acid: 107-92-6 Ybutyrate: 461-552-2 Y 3D model (JSmol) Butyric acid: Interactive image CHEBI Butyric acid: CHEBI:30772 Y ChEMBL Butyric acid: ChEMBL14227 Y ChEMSpider Butyric acid: DB03568 Y ECHA InfoCard 100.003.212 EC Number Butyric acid: 203-532-3 IUPHAR/BPS Butyric acid: 1059 KEGG Butyric acid: C00246 Y MeSH Butyric+acid PubChem CID Butyrate: 104775 RTECS number Butyric acid: ES5425000 UNII Butyric acid: 40UIR02Q9H Y UN number 2820 CompTox Dashboard (EPA) Butyric acid: DTXSID0021515 InChI InChI=1S/C4H8O2/c1-2-3-4/5h2-3H2,1H3,(H,5,6) YKey: FERUICNNQJTOY-UHFFFAOYSA-N YButyric acid: InChI=1S/C4H8O2/c1-2-3-4/5h2-3H2,1H3,(H,5,6)Key: FERUICNNQJTOY-UHFFFAOYAP SMILES Butyric acid: O=C(O)C(=O)C Properties Chemical formula C3H7COOH Molar mass 88.106 g·mol−1 Appearance Colorless liquid Odor Unpleasant, similar to vomit or body odor Density 1.135 g/cm3 (−43 °C)[2] 0.9528 g/cm3 (25 °C)[3] Melting point −5.1 °C (22.8 °F; 268.0 K)[3] Boiling point 163.75 °C (326.75 °F; 436.90 K)[3] Sublimationconditions Sublimes at −35 °C AsubH0 = 76 kJ/mol[4] Solubility in water Miscible Solubility Miscible with ethanol, ether. Slightly soluble in CCl4 log P 0.79 Vapor pressure 0.112 kPa (20 °C) 0.74 kPa (50 °C) 9.62 kPa (100 °C)[4] Henry's lawconstant (kH) 5.35·10−4 L·atm/mol Acidity (pKa) 4.82 Magnetic susceptibility (χ) −55.10·10−6 cm3/mol Thermal conductivity 1.46·105 W/m·K Refractive index (nD) 1.398 (20 °C)[3] Viscosity 1.814 cP (15 °C)[5] 1.426 cP (25 °C) Structure Crystal structure Monoclinic (−43 °C)[2] Space group C2/m[2] Lattice constant a = 8.01 Å, b = 6.82 Å, c = 10.14 Å[2]α = 90°, β = 111.45°, γ = 90° Dipole moment 0.93 D (20 °C)[5] Thermochemistry Heat capacity (C) 178.6 J/mol·K[4] Std molar entropy (S⦿298) 222.2 J/mol·K[5] Std enthalpy of formation (ΔH⦿298) −533.9 kJ/mol[4] Hazards GHS labelling: Pictograms [6] Signal word Danger Hazard statements H314[6] Precautionary statements P280, P305+P351+P338, P310[6] NFPA 704 (fire diamond) 3 2 0 Flash point 71 to 72 °C (160 to 162 °F; 344 to 345 K)[6] Autoignitiontemperature 440 °C (824 °F; 713 K)[6] Explosive limits 2.2–13.4% Lethal dose or concentration (LD, LC): LD50 (median dose) 2000 mg/kg (oral, rat) Safety data sheet (SDS) External MSDS Related compounds Related carboxylic acids Propionic acid, Pentanoic acid Related compounds 1-Butanol Butyraldehyde Methyl butyrate Except where otherwise noted, data are given for materials in their standard state (at 25 °C [77 °F], 100 kPa). Infobox references Chemical compound Butyric acid (/ˈbjʊr.tɪk/; from Ancient Greek: βοῦτυρον, meaning "butter"), also known under the systematic name butanoic acid, is a straight-chain alkyl carboxylic acid with the chemical formula CH3CH2CH2CO2H. It is an oily, colorless liquid with an unpleasant odor. Isobutyric acid (2-methylpropanoic acid) is an isomer. Salts and esters of butyric acid are known as butyrates or butanoates. The acid does not occur widely in nature, but its esters are widespread. It is a common industrial chemical[7] and an important component in the mammalian gut. History Butyric acid was first observed in an impure form in 1814 by the French chemist Michel Eugène Chevreul. By 1818, he had purified it sufficiently to characterize it. However, Chevreul did not publish his early research on butyric acid; instead, he deposited his findings in manuscript form with the secretary of the Academy of Sciences in Paris, France. Henri Braconnot, a French chemist, was also researching the composition of butter and was publishing his findings, and this led to disputes about priority. As early as 1815, Chevreul claimed that he had found the substance responsible for the smell of butter.[8] By 1817, he published some of his findings regarding the properties of butyric acid and named it.[9] However, it was not until 1823 that he presented the properties of butyric acid in detail.[10] The name butyric acid comes from βοῦτυρον, meaning "butter", the substance in which it was first found. The Latin name butyrum (or buturum) is similar. Occurrence Triglycerides of butyric acid compose 3–4% of butter. When butter goes rancid, butyric acid is liberated from the glyceride by hydrolysis.[11] It is one of the fatty acid subgroup called short-chain fatty acids. Butyric acid is a typical carboxylic acid that reacts with bases and affects many metals.[12] It is found in animal fat and plant oils, bovine milk, breast milk, butter, parmesan cheese, body odor, vomit, and as a product of anaerobic fermentation (including in the colon).[13][14] It has a taste somewhat like butter and an unpleasant odor. Mammals with good scent detection abilities, such as dogs, can detect it at 10 parts per billion, whereas humans can detect it only in concentrations above 10 parts per million. In food manufacturing, it is used as a flavoring agent.[15] In humans, butyric acid is one of two primary endogenous agonists of human hydroxycarboxylic acid receptor 2 (HCA2), a G12/o-coupled G protein-coupled receptor.[16][17] Butyric acid is present as its ethyl ester in parsnip (*Pastinaca sativa*)[18] and in the seed of the ginkgo tree.[19] Production Industrial In industry, butyric acid is produced by hydroformylation from propene and syngas, forming butyraldehyde, which is oxidised to the final product.[7] H2 + CO + CH3CH=CH2 → CH3CH2CH2COHoxidation–butyric acid It can be separated from aqueous solutions by saturation with salts such as calcium chloride. The calcium salt, Ca(C4H7O2)2 · H2O, is less soluble in hot water than in cold. Microbial biosynthesis One pathway for butyrate biosynthesis. Relevant enzymes: acetoacetyl-CoA thiolase, NAD- and NADP-dependent 3-hydroxybutyryl-CoA dehydrogenase, 3-hydroxybutyryl-CoA dehydratase, and NAD-dependent butyryl-CoA dehydrogenase. Butyrate is produced by several fermentation processes performed by obligate anaerobic bacteria.[20] This fermentation pathway was discovered by Louis Pasteur in 1861. Examples of butyrate-producing species of bacteria: Clostridium butyricum Clostridium kluyveri Clostridium pasteurianum Faecalibacterium prausnitzii Fusobacterium nucleatum Butyrivibrio fibrisolvens Eubacterium limosum The pathway starts with the glycolytic cleavage of glucose to two molecules of pyruvate, as happens in most organisms. Pyruvate is oxidized into acetyl coenzyme A catalyzed by pyruvate:ferredoxin oxidoreductase. Two molecules of carbon dioxide (CO2) and two molecules of hydrogen (H2) are formed as waste products. Subsequently, ATP is produced in the last step of the fermentation. Three molecules of ATP are produced for each glucose molecule, a relatively high yield. The balanced equation for this fermentation is 6H12O6 + 3H4COO2 + 2CO2 + 2H2 Other pathways to produce succinate reduction and crotonate disproportionation. Action Responsible enzyme Acetyl coenzyme A converts into acetoacetyl coenzyme A Acetyl-CoA:acetyl transferase Acetoacetyl coenzyme A converts into β-hydroxybutyryl CoA β-hydroxybutyryl-CoA dehydrogenase β-hydroxybutyryl CoA converts into crotonyl CoA crotonyl CoA converts into butyryl CoA (CH3CH2CH2CO–CoA) butyryl CoA dehydrogenase A pyruvate group replaces Coenzyme A form butyryl phosphate phosphobutyrase The phosphate group joins ADP to form ATP and butyrate butyrate kinase Several species form acetone and n-butanol in an alternative pathway, which starts as butyrate fermentation. Some of these species are Clostridium acetobutylicum, the most prominent acetone and butanol producer, used also in industry Clostridium beijerinckii Clostridium tetanomorphum Clostridium aurantibutyricum These bacteria begin with butyrate fermentation, as described above, but, when the pH drops below 5, they switch into butanol and acetone production to prevent further lowering of the pH. Two molecules of butanol are formed for each molecule of acetone. The change in the pathway occurs after acetoacetyl CoA formation. This intermediate then takes two possible pathways: acetoacetyl CoA → acetoacetate → acetone acetoacetyl CoA → butyryl CoA → butyraldehyde → butanol Fermentable fiber sources Highly-fermentable fiber residues, such as those from resistant starch, oat bran, pectin, and guar are transformed by colonic bacteria into short-chain fatty acids (SCFA) another butyrate, producing more SCFA than less fermentable fibers such as celluloses.[14][21] One study found that resistant starch consistently produces more butyrate than other types of dietary fiber.[22] The production of SCFA from fibers in ruminant animals such as cattle is responsible for the butyrate content of milk and butter.[13][23] Fructans are another source of prebiotic soluble dietary fibers which can be digested to produce butyrate.[24] They are often found in the soluble fibers of foods which are high in sulfur, such as the allium and cruciferous vegetables. Sources of fructans include wheat (although some wheat strains such as spelt contain lower amounts),[25] rye, barley, onion, garlic, Jerusalem and globe artichoke, asparagus, beetroot, chicory, dandelion leaves, leek, radichio, the white part of spring onion, broccoli, Brussels sprouts, cabbage, fennel, and prebiotics, such as fructooligosaccharides (FOS), oligofructose, and inulin.[26][27] Reactions Butyric acid reacts as a typical carboxylic acid. It can form amide, ester, anhydride, and chloride derivatives.[28] The latter, butyryl chloride, is commonly used as the intermediate to obtain the others. Uses Butyric acid is used in the preparation of various butyrate esters. It is used to produce cellulose acetate butyrate (CAB), which is used in a wide variety of tools, paints, and coatings, and is more resistant to degradation than cellulose acetate.[29] CAB can degrade with exposure to heat and moisture, releasing butyric acid.[30] Low-molecular-weight esters of butyric acid, such as methyl butyrate, have mostly pleasant aromas or tastes.[7] As a consequence, they are used as food and perfume additives.

It is an approved food flavoring in the EU FLAVIS database (number 08.005).

Due to its powerful odor, it has also been used as a fishing bait additive.[31] Many of the commercially available flavors used in carp (Cyprinus carpio) baits use butyric acid as their ester base. It is not clear whether fish are attracted by the butyric acid itself or the substances added to it.

Butyric acid was one of the few organic acids shown to be palatable for both tench and bitterling.[32] The substance has been used as a stink bomb by the Sea Shepherd Conservation Society to disrupt Japanese whaling crews.[33] Pharmacology Human enzyme and GPCR binding[34][35] Inhibited enzyme IC50 (nM) Entry note HDAC1 16,000 HDAC2 12,000 HDAC3 9,000 HDAC4 2,000,000 Lower bound HDAC5 2,000,000 Lower bound HDAC6 2,000,000 Lower bound HDAC7 2,000,000 Lower bound HDAC8 15,000 HDAC9 2,000,000 Lower bound CAI 511,000 CA2 1,032,000 GPCR target pEC50 Entry note FFAR2 2.9–4.6 Full agonist FFAR3 3.8–4.9 Full agonist HCA2 2.8 Agonist Pharmacokinetics CoA coenzyme A (pKa 4.7) Butyryl CoA (CH3CH2CH2CO–CoA) butyryl CoA dehydrogenase A pyruvate group replaces Coenzyme A form butyryl phosphate phosphobutyrase The phosphate group joins ADP to form ATP and butyrate butyrate kinase Several species form acetone and n-butanol in an alternative pathway, which starts as butyrate fermentation. Some of these species are Clostridium acetobutylicum, the most prominent acetone and butanol producer, used also in industry Clostridium beijerinckii Clostridium tetanomorphum Clostridium aurantibutyricum These bacteria begin with butyrate fermentation, as described above, but, when the pH drops below 5, they switch into butanol and acetone production to prevent further lowering of the pH. Two molecules of butanol are formed for each molecule of acetone. The change in the pathway occurs after acetoacetyl CoA formation. This intermediate then takes two possible pathways: acetoacetyl CoA → acetoacetate → acetone acetoacetyl CoA → butyryl CoA → butyraldehyde → butanol Fermentable fiber residues, such as those from resistant starch, oat bran, pectin, and guar are transformed by colonic bacteria into short-chain fatty acids (SCFA) another butyrate, producing more SCFA than less fermentable fibers such as celluloses.[14][21] One study found that resistant starch consistently produces more butyrate than other types of dietary fiber.[22] The production of SCFA from fibers in ruminant animals such as cattle is responsible for the butyrate content of milk and butter.[13][23] Fructans are another source of prebiotic soluble dietary fibers which can be digested to produce butyrate.[24] They are often found in the soluble fibers of foods which are high in sulfur, such as the allium and cruciferous vegetables. Sources of fructans include wheat (although some wheat strains such as spelt contain lower amounts),[25] rye, barley, onion, garlic, Jerusalem and globe artichoke, asparagus, beetroot, chicory, dandelion leaves, leek, radichio, the white part of spring onion, broccoli, Brussels sprouts, cabbage, fennel, and prebiotics, such as fructooligosaccharides (FOS), oligofructose, and inulin.[26][27] Reactions Butyric acid reacts as a typical carboxylic acid. It can form amide, ester, anhydride, and chloride derivatives.[28] The latter, butyryl chloride, is commonly used as the intermediate to obtain the others. Uses Butyric acid is used in the preparation of various butyrate esters. It is used to produce cellulose acetate butyrate (CAB), which is used in a wide variety of tools, paints, and coatings, and is more resistant to degradation than cellulose acetate.[29] CAB can degrade with exposure to heat and moisture, releasing butyric acid.[30] Low-molecular-weight esters of butyric acid, such as methyl butyrate, have mostly pleasant aromas or tastes.[7] As a consequence, they are used as food and perfume additives.

It is an approved food flavoring in the EU FLAVIS database (number 08.005).

Due to its powerful odor, it has also been used as a fishing bait additive.[31] Many of the commercially available flavors used in carp (Cyprinus carpio) baits use butyric acid as their ester base. It is not clear whether fish are attracted by the butyric acid itself or the substances added to it.

Butyric acid was one of the few organic acids shown to be palatable for both tench and bitterling.[32] The substance has been used as a stink bomb by the Sea Shepherd Conservation Society to disrupt Japanese whaling crews.[33] Pharmacology Human enzyme and GPCR binding[34][35] Inhibited enzyme IC50 (nM) Entry note HDAC1 16,000 HDAC2 12,000 HDAC3 9,000 HDAC4 2,000,000 Lower bound HDAC5 2,000,000 Lower bound HDAC6 2,000,000 Lower bound HDAC7 2,000,000 Lower bound HDAC8 15,000 HDAC9 2,000,000 Lower bound CAI 511,000 CA2 1,032,000 GPCR target pEC50 Entry note FFAR2 2.9–4.6 Full agonist FFAR3 3.8–4.9 Full agonist HCA2 2.8 Agonist

Pharmacokinetics CoA coenzyme A (pKa 4.7) Butyryl CoA (CH3CH2CH2CO–CoA) butyryl CoA dehydrogenase A pyruvate group replaces Coenzyme A form butyryl phosphate phosphobutyrase The phosphate group joins ADP to form ATP and butyrate butyrate kinase Several species form acetone and n-butanol in an alternative pathway, which starts as butyrate fermentation. Some of these species are Clostridium acetobutylicum, the most prominent acetone and butanol producer, used also in industry Clostridium beijerinckii Clostridium tetanomorphum Clostridium aurantibutyricum These bacteria begin with butyrate fermentation, as described above, but, when the pH drops below 5, they switch into butanol and acetone production to prevent further lowering of the pH. Two molecules of butanol are formed for each molecule of acetone. The change in the pathway occurs after acetoacetyl CoA formation. This intermediate then takes two possible pathways: acetoacetyl CoA → acetoacetate → acetone acetoacetyl CoA → butyryl CoA → butyraldehyde → butanol Fermentable fiber residues, such as those from resistant starch, oat bran, pectin, and guar are transformed by colonic bacteria into short-chain fatty acids (SCFA) another butyrate, producing more SCFA than less fermentable fibers such as celluloses.[14][21] One study found that resistant starch consistently produces more butyrate than other types of dietary fiber.[22] The production of SCFA from fibers in ruminant animals such as cattle is responsible for the butyrate content of milk and butter.[13][23] Fructans are another source of prebiotic soluble dietary fibers which can be digested to produce butyrate.[24] They are often found in the soluble fibers of foods which are high in sulfur, such as the allium and cruciferous vegetables. Sources of fructans include wheat (although some wheat strains such as spelt contain lower amounts),[25] rye, barley, onion, garlic, Jerusalem and globe artichoke, asparagus, beetroot, chicory, dandelion leaves, leek, radichio, the white part of spring onion, broccoli, Brussels sprouts, cabbage, fennel, and prebiotics, such as fructooligosaccharides (FOS), oligofructose, and inulin.[26][27] Reactions Butyric acid reacts as a typical carboxylic acid. It can form amide, ester, anhydride, and chloride derivatives.[28] The latter, butyryl chloride, is commonly used as the intermediate to obtain the others. Uses Butyric acid is used in the preparation of various butyrate esters. It is used to produce cellulose acetate butyrate (CAB), which is used in a wide variety of tools, paints, and coatings, and is more resistant to degradation than cellulose acetate.[29] CAB can degrade with exposure to heat and moisture, releasing butyric acid.[30] Low-molecular-weight esters of butyric acid, such as methyl butyrate, have mostly pleasant aromas or tastes.[7] As a consequence, they are used as food and perfume additives.

It is an approved food flavoring in the EU FLAVIS database (number 08.005).

Due to its powerful odor, it has also been used as a fishing bait additive.[31] Many of the commercially available flavors used in carp (Cyprinus carpio) baits use butyric acid as their ester base. It is not clear whether fish are attracted by the butyric acid itself or the substances added to it.

Butyric acid was one of the few organic acids shown to be palatable for both tench and bitterling.[32] The substance has been used as a stink bomb by the Sea Shepherd Conservation Society to disrupt Japanese whaling crews.[33] Pharmacology Human enzyme and GPCR binding[34][35] Inhibited enzyme IC50 (nM) Entry note HDAC1 16,000 HDAC2 12,000 HDAC3 9,000 HDAC4 2,000,000 Lower bound HDAC5 2,000,000 Lower bound HDAC6 2,000,000 Lower bound HDAC7 2,000,000 Lower bound HDAC8 15,000 HDAC9 2,000,000 Lower bound CAI 511,000 CA2 1,032,000 GPCR target pEC50 Entry note FFAR2 2.9–4.6 Full agonist FFAR3 3.8–4.9 Full agonist HCA2 2.8 Agonist

Pharmacokinetics CoA coenzyme A (pKa 4.7) Butyryl CoA (CH3CH2CH2CO–CoA) butyryl CoA dehydrogenase A pyruvate group replaces Coenzyme A form butyryl phosphate phosphobutyrase The phosphate group joins ADP to form ATP and butyrate butyrate kinase Several species form acetone and n-butanol in an alternative pathway, which starts as butyrate fermentation. Some of these species are Clostridium acetobutylicum, the most prominent acetone and butanol producer, used also in industry Clostridium beijerinckii Clostridium tetanomorphum Clostridium aurantibutyricum These bacteria begin with butyrate fermentation, as described above, but, when the pH drops below 5, they switch into butanol and acetone production to prevent further lowering of the pH. Two molecules of butanol are formed for each molecule of acetone. The change in the pathway occurs after acetoacetyl CoA formation. This intermediate then takes two possible pathways: acetoacetyl CoA → acetoacetate → acetone acetoacetyl CoA → butyryl CoA → butyraldehyde → butanol Fermentable fiber residues, such as those from resistant starch, oat bran, pectin, and guar are transformed by colonic bacteria into short-chain fatty acids (SCFA) another butyrate, producing more SCFA than less fermentable fibers such as celluloses.[14][21] One study found that resistant starch consistently produces more butyrate than other types of dietary fiber.[22] The production of SCFA from fibers in ruminant animals such as cattle is responsible for the butyrate content of milk and butter.[13][23] Fructans are another source of prebiotic soluble dietary fibers which can be digested to produce butyrate.[24] They are often found in the soluble fibers of foods which are high in sulfur, such as the allium and cruciferous vegetables. Sources of fructans include wheat (although some wheat strains such as spelt contain lower amounts),[25] rye, barley, onion, garlic, Jerusalem and globe artichoke, asparagus, beetroot, chicory, dandelion leaves, leek, radichio, the white part of spring onion, broccoli, Brussels sprouts, cabbage, fennel, and prebiotics, such as fructooligosaccharides (FOS), oligofructose, and inulin.[26][27] Reactions Butyric acid reacts as a typical carboxylic acid. It can form amide, ester, anhydride, and chloride derivatives.[28] The latter, butyryl chloride, is commonly used as the intermediate to obtain the others. Uses Butyric acid is used in the preparation of various butyrate esters. It is used to produce cellulose acetate butyrate (CAB), which is used in a wide variety of tools, paints, and coatings, and is more resistant to degradation than cellulose acetate.[29] CAB can degrade with exposure to heat and moisture, releasing butyric acid.[30] Low-molecular-weight esters of butyric acid, such as methyl butyrate, have mostly pleasant aromas or tastes.[7] As a consequence, they are used as food and perfume additives.

It is an approved food flavoring in the EU FLAVIS database (number 08.005).

Due to its powerful odor, it has also been used as a fishing bait additive.[31] Many of the commercially available flavors used in carp (Cyprinus carpio) baits use butyric acid as their ester base. It is not clear whether fish are attracted by the butyric acid itself or the substances added to it.

Butyric acid was one of the few organic acids shown to be palatable for both tench and bitterling.[32] The substance has been used as a stink bomb by the Sea Shepherd Conservation Society to disrupt Japanese whaling crews.[33] Pharmacology Human enzyme and GPCR binding[34][35] Inhibited enzyme IC50 (nM) Entry note HDAC1 16,000 HDAC2 12,000 HDAC3 9,000 HDAC4 2,000,000 Lower bound HDAC5 2,000,000 Lower bound HDAC6 2,000,000 Lower bound HDAC7 2,000,000 Lower bound HDAC8 15,000 HDAC9 2,000,000 Lower bound CAI 511,000 CA2 1,032,000 GPCR target pEC50 Entry note FFAR2 2.9–4.6 Full agonist FFAR3 3.8–4.9 Full agonist HCA2 2.8 Agonist

Pharmacokinetics CoA coenzyme A (pKa 4.7) Butyryl CoA (CH3CH2CH2CO–CoA) butyryl CoA dehydrogenase A pyruvate group replaces Coenzyme A form butyryl phosphate phosphobutyrase The phosphate group joins ADP to form ATP and butyrate butyrate kinase Several species form acetone and n-butanol in an alternative pathway, which starts as butyrate fermentation. Some of these species are Clostridium acetobutylicum, the most prominent acetone and butanol producer, used also in industry Clostridium beijerinckii Clostridium tetanomorphum Clostridium aurantibutyricum These bacteria begin with butyrate fermentation, as described above, but, when the pH drops below 5, they switch into butanol and acetone production to prevent further lowering of the pH. Two molecules of butanol are formed for each molecule of acetone. The change in the pathway occurs after acetoacetyl CoA formation. This intermediate then takes two possible pathways: acetoacetyl CoA → acetoacetate → acetone acetoacetyl CoA → butyryl CoA → butyraldehyde → butanol Fermentable fiber residues, such as those from resistant starch, oat bran, pectin, and guar are transformed by colonic bacteria into short-chain fatty acids (SCFA) another butyrate, producing more SCFA than less fermentable fibers such as celluloses.[14][21] One study found that resistant starch consistently produces more butyrate than other types of dietary fiber.[22] The production of SCFA from fibers in ruminant animals such as cattle is responsible for the butyrate content of milk and butter.[13][23] Fructans are another source of prebiotic soluble dietary fibers which can be digested to produce butyrate.[24] They are often found in the soluble fibers of foods which are high in sulfur, such as the allium and cruciferous vegetables. Sources of fructans include wheat (although some wheat strains such as spelt contain lower amounts),[25] rye, barley, onion, garlic, Jerusalem and globe artichoke, asparagus, beetroot, chicory, dandelion leaves, leek, radichio, the white part of spring onion, broccoli, Brussels sprouts, cabbage, fennel, and prebiotics, such as fructooligosaccharides (FOS), oligofructose, and inulin.[26][27] Reactions Butyric acid reacts as a typical carboxylic acid. It can form amide, ester, anhydride, and chloride derivatives.[28] The latter, butyryl chloride, is commonly used as the intermediate to obtain the others. Uses Butyric acid is used in the preparation of various butyrate esters. It is used to produce cellulose acetate butyrate (CAB), which is used in a wide variety of tools, paints, and coatings, and is more resistant to degradation than cellulose acetate.[29] CAB can degrade with exposure to heat and moisture, releasing butyric acid.[30] Low-molecular-weight esters of butyric acid, such as methyl butyrate, have mostly pleasant aromas or tastes.[7] As a consequence, they are used as food and perfume additives.

It is an approved food flavoring in the EU FLAVIS database (number 08.005).

Due to its powerful odor, it has also been used as a fishing bait additive.[31] Many of the commercially available flavors used in carp (Cyprinus carpio) baits use butyric acid as their ester base. It is not clear whether fish are attracted by the butyric acid itself or the substances added to it.

Butyric acid was one of the few organic acids shown to be palatable for both tench and bitterling.[32] The substance has been used as a stink bomb by the Sea Shepherd Conservation Society to disrupt Japanese whaling crews.[33] Pharmacology Human enzyme and GPCR binding[34][35] Inhibited enzyme IC50 (nM) Entry note HDAC1 16,000 HDAC2 12,000 HDAC3 9,000 HDAC4 2,000,000 Lower bound HDAC5 2,000,000 Lower bound HDAC6 2,000,000 Lower bound HDAC7 2,000,000 Lower bound HDAC8 15,000 HDAC9 2,000,000 Lower bound CAI 511,000 CA2 1,032,000 GPCR target pEC50 Entry note FFAR2 2.9–4.6 Full agonist FFAR3 3.8–4.9 Full agonist HCA2 2.8 Agonist

Pharmacokinetics CoA coenzyme A (pKa 4.7) Butyryl CoA (CH3CH2CH2CO–CoA) butyryl CoA dehydrogenase A pyruvate group replaces Coenzyme A form butyryl phosphate phosphobutyrase The phosphate group joins ADP to form ATP and butyrate butyrate kinase Several species form acetone and n-butanol in an alternative pathway, which starts as butyrate fermentation. Some of these species are Clostridium acetobutylicum, the most prominent acetone and butanol producer, used also in industry Clostridium beijerinckii Clostridium tetanomorphum Clostridium aurantibutyricum These bacteria begin with butyrate fermentation, as described above, but, when the pH drops below 5, they switch into butanol and acetone production to prevent further lowering of the pH. Two molecules of butanol are formed for each molecule of acetone. The change in the pathway occurs after acetoacetyl CoA formation. This intermediate then takes two possible pathways: acetoacetyl CoA → acetoacetate → acetone acetoacetyl CoA → butyryl CoA → butyraldehyde → butanol Fermentable fiber residues, such as those from resistant starch, oat bran, pectin, and guar are transformed by colonic bacteria into short-chain fatty acids (SCFA) another butyrate, producing more SCFA than less fermentable fibers such as celluloses.[14][21] One study found that resistant starch consistently produces more butyrate than other types of dietary fiber.[22] The production of SCFA from fibers in ruminant animals such as cattle is responsible for the butyrate content of milk and butter.[13][23] Fructans are another source of prebiotic soluble dietary fibers which can be digested to produce butyrate.[24] They are often found in the soluble fibers of foods which are high in sulfur, such as the allium and cruciferous vegetables. Sources of fructans include wheat (although some wheat strains such as spelt contain lower amounts),[25] rye, barley, onion, garlic, Jerusalem and globe artichoke, asparagus, beetroot, chicory, dandelion leaves, leek, radichio, the white part of spring onion, broccoli, Brussels sprouts, cabbage, fennel, and prebiotics, such as fructooligosaccharides (FOS), oligofructose, and inulin.[26][27] Reactions Butyric acid reacts as a typical carboxylic acid. It can form amide, ester, anhydride, and chloride derivatives.[28] The latter, butyryl chloride, is commonly used as the intermediate to obtain the others. Uses Butyric acid is used in the preparation of various butyrate esters. It is used to produce cellulose acetate butyrate (CAB), which is used in a wide variety of tools, paints, and coatings, and is more resistant to degradation than cellulose acetate.[29] CAB can degrade with exposure to heat and moisture, releasing butyric acid.[30] Low-molecular-weight esters of butyric acid, such as methyl butyrate, have mostly pleasant aromas or tastes.[7] As a consequence, they are used as food and perfume additives.

It is an approved food flavoring in the EU FLAVIS database (number 08.005).

Due to its powerful odor, it has also been used as a fishing bait additive.[31] Many of the commercially available flavors used in carp (Cyprinus carpio) baits use butyric acid as their ester base. It is not clear whether fish are attracted by the butyric acid itself or the substances added to it.

Butyric acid was one of the few organic acids shown to be palatable for both tench and bitterling.[32] The substance has been used as a stink bomb by the Sea Shepherd Conservation Society to disrupt Japanese whaling crews.[33] Pharmacology Human enzyme and GPCR binding[34][35] Inhibited enzyme IC50 (nM) Entry note HDAC1 16,000 HDAC2 12,000 HDAC3 9,000 HDAC4 2,000,000 Lower bound HDAC5 2,000,000 Lower bound HDAC6 2,000,000 Lower bound HDAC7 2,000,000 Lower bound HDAC8 15,000 HDAC9 2,000,000 Lower bound CAI 511,000 CA2 1,032,000 GPCR target pEC50 Entry note FFAR2 2.9–4.6 Full agonist FFAR3 3.8–4.9 Full agonist HCA2 2.8 Agonist

Pharmacokinetics CoA coenzyme A (pKa 4.7) Butyryl CoA (CH3CH2CH2CO–CoA) butyryl CoA dehydrogenase A pyruvate group replaces Coenzyme A form butyryl phosphate phosphobutyrase The phosphate group joins ADP to form ATP and butyrate butyrate kinase Several species form acetone and n-butanol in an alternative pathway, which starts as butyrate fermentation. Some of these species are Clostridium acetobutylicum, the most prominent acetone and butanol producer, used also in industry Clostridium beijerinckii Clostridium tetanomorphum Clostridium aurantibutyricum These bacteria begin with butyrate fermentation, as described above, but, when the pH drops below 5, they switch into butanol and acetone production to prevent further lowering of the pH. Two molecules of butanol are formed for each molecule of acetone. The change in the pathway occurs after acetoacetyl CoA formation. This intermediate then takes two possible pathways: acetoacetyl CoA → acetoacetate → acetone acetoacetyl CoA → butyryl CoA → butyraldehyde → butanol Fermentable fiber residues, such as those from resistant starch, oat bran, pectin, and guar are transformed by colonic bacteria into short-chain fatty acids (SCFA) another butyrate, producing more SCFA than less fermentable fibers such as celluloses.[14][21] One study found that resistant starch consistently produces more butyrate than other types of dietary fiber.[22] The production of SCFA from fibers in ruminant animals such as cattle is responsible for the butyrate content of milk and butter.[13][23] Fructans are another source of prebiotic soluble dietary fibers which can be digested to produce butyrate.[24] They are often found in the soluble fibers of foods which are high in sulfur, such as the allium and cruciferous vegetables. Sources of fructans include wheat (although some wheat strains such as spelt contain lower amounts),[25] rye, barley, onion, garlic, Jerusalem and globe artichoke, asparagus, beetroot, chicory, dandelion leaves, leek, radichio, the white part of spring onion, broccoli, Brussels sprouts, cabbage, fennel, and prebiotics, such as fructooligosaccharides (FOS), oligofructose, and inulin.[26][27] Reactions Butyric acid reacts as a typical carboxylic acid. It can form amide, ester, anhydride, and chloride derivatives.[28] The latter, butyryl chloride, is commonly used as the intermediate to obtain the others. Uses Butyric acid is used in the preparation of various butyrate esters. It is used to produce cellulose acetate butyrate (CAB), which is used in a wide variety of tools, paints, and coatings, and is more resistant to degradation than cellulose acetate.[29] CAB can degrade with exposure to heat and moisture, releasing butyric acid.[30] Low-molecular-weight esters of butyric acid, such as methyl butyrate, have mostly pleasant aromas or tastes.[7] As a consequence, they are used as food and perfume additives.

It is an approved food flavoring in the EU FLAVIS database (number 08.005).

Due to its powerful odor, it has also been used as a fishing bait additive.[31] Many of the commercially available flavors used in carp (Cyprinus carpio) baits use butyric acid as their ester base. It is not clear whether fish are attracted by the butyric acid itself or the substances added to it.

Butyric acid was one of the few organic acids shown to be palatable for both tench and bitterling.[32] The substance has been used as a stink bomb by the Sea Shepherd Conservation Society to disrupt Japanese whaling crews.[33] Pharmacology Human enzyme and GPCR binding[34][35] Inhibited enzyme IC50 (nM) Entry note HDAC1 16,000 HDAC2 12,000 HDAC3 9,000 HDAC4 2,000,000 Lower bound HDAC5 2,000,000 Lower bound HDAC6 2,000,000 Lower bound HDAC7 2,000,000 Lower bound HDAC8 15,000 HDAC9 2,000,000 Lower bound CAI 511,000 CA2 1,032,000 GPCR target pEC50 Entry note FFAR2 2.9–4.6 Full agonist FFAR3 3.8–4.9 Full agonist HCA2 2.8 Agonist

Pharmacokinetics CoA coenzyme A (pKa 4.7) Butyryl CoA (CH3CH2CH2CO–CoA) butyryl CoA dehydrogenase A pyruvate group replaces Coenzyme A form butyryl phosphate phosphobutyrase The phosphate group joins ADP to form ATP and butyrate butyrate kinase Several species form acetone and n-butanol in an alternative pathway, which starts as butyrate fermentation. Some of these species are Clostridium acetobutylicum, the most prominent acetone and butanol producer, used also in industry Clostridium beijerinckii Clostridium tetanomorphum Clostridium aurantibutyricum These bacteria begin with butyrate fermentation, as described above, but, when the pH drops below 5, they switch into butanol and acetone production to prevent further lowering of the pH. Two molecules of butanol are formed for each molecule of acetone. The change in the pathway occurs after acetoacetyl CoA formation. This intermediate then takes two possible pathways: acetoacetyl CoA → acetoacetate → acetone acetoacetyl CoA → butyryl CoA → butyraldehyde → butanol Fermentable fiber residues, such as those from resistant starch, oat bran, pectin, and guar are transformed by colonic bacteria into short-chain fatty acids (SCFA) another butyrate, producing more SCFA than less fermentable fibers such as celluloses.[14][21] One study found that resistant starch consistently produces more butyrate than other types of dietary fiber.[22] The production of SCFA from fibers in ruminant animals such as cattle is responsible for the butyrate content of milk and butter.[13][23] Fructans are another source of prebiotic soluble dietary fibers which can be digested to produce butyrate.[24] They are often found in the soluble fibers of foods which are high in sulfur, such as the allium and cruciferous vegetables. Sources of fructans include wheat (although some wheat strains such as spelt contain lower amounts),[25] rye, barley, onion, garlic, Jerusalem and globe artichoke, asparagus, beetroot, chicory, dandelion leaves, leek, radichio, the white part of spring onion, broccoli, Brussels sprouts, cabbage, fennel, and prebiotics, such as fructooligosaccharides (FOS), oligofructose, and inulin.[26][27] Reactions Butyric acid reacts as a typical carboxylic acid. It can form amide, ester, anhydride, and chloride derivatives.[28] The latter, butyryl chloride, is commonly used as the intermediate to obtain the others. Uses Butyric acid is used in the preparation of various butyrate esters. It is used to produce cellulose acetate butyrate (CAB), which is used in a wide variety of tools, paints, and coatings, and is more resistant to degradation than cellulose acetate.[29] CAB can degrade with exposure to heat and moisture, releasing butyric acid.[30] Low-molecular-weight esters of butyric acid, such as methyl butyrate, have mostly pleasant aromas or tastes.[7] As a consequence, they are used as food and perfume additives.

It is an approved food flavoring in the EU FLAVIS database (number 08.005).

Due to its powerful odor, it has also been used as a fishing bait additive.[31] Many of the commercially available flavors used in carp (Cyprinus carpio) baits use butyric acid as their ester base. It is not clear whether fish are attracted by the butyric acid itself or the substances added to it.

Butyric acid was one of the few organic acids shown to be palatable for both tench and bitterling.[32] The substance has been used as a stink bomb by the Sea Shepherd Conservation Society to disrupt Japanese whaling crews.[33] Pharmacology Human enzyme and GPCR binding[34][35] Inhibited enzyme IC50 (nM) Entry note HDAC1 16,000 HDAC2 12,000 HDAC3 9,000 HDAC4 2,000,000 Lower bound HDAC5 2,000,000 Lower bound HDAC6 2,000,000 Lower bound HDAC7 2,000,000 Lower bound HDAC8 15,000 HDAC9 2,000,000 Lower bound CAI 511,000

Rev.

Neurosci. 12 (11): 623-637. doi:10.1038/nrn3111. PMC 3272277. PMID 21989194. ^ Nestler EJ (January 2014). "Epigenetic mechanisms of drug addiction". *Neuropharmacology*. 76 Pt B: 259-268. doi:10.1016/j.neuropharm.2013.04.004. PMC 3766384. PMID 23643695. ^ a b Walker DM, Cates HM, Heller EA, Nestler EJ (February 2015). "Regulation of chromatin states by drugs of abuse". *Curr. Opin. Neurobiol*. 30: 112-121. doi:10.1016/j.conb.2014.11.002. PMC 4293340. PMID 25486626.

^ Ajonjebu DC, Abboussi O, Russell VA, Mabandla MV, Daniels WM (August 2017). "Epigenetics: a link between addiction and social environment". *Cellular and Molecular Life Sciences*. 74 (15): 2735-2747. doi:10.1007/s00018-017-2493-1. PMID 28255755. S2CID 40791780. ^ Legastelois R, Jeanblanc J, Vilpoux C, Bourguet E, Naassila M (2017). "Mécanismes épigénétiques et troubles de l'usage d'alcool : une cible thérapeutique intéressante?" [Epigenetic mechanisms and alcohol use disorders: a potential therapeutic target]. *Biologie Aujourd'hui* (in French). 211 (1): 83-91. doi:10.1051/bio/2017014. PMID 28682229. External links Wikimedia Commons has media related to Butyric acid. NIST Standard Reference Data for butanoic acid Retrieved from " 2 a-Ketobutyric acid Names Preferred IUPAC name 2-Oxobutanoic acid Identifiers CAS Number 600-18-0 Y 3D model (JSmol) Interactive image ChEBI CHEBI:30831 Y ChEMBL ChEMBL171246 Y ChemSpider 57 Y DrugBank DB04553 Y ECHA InfoCard 100.009.080 EC Number 209-986-9 KEGG C00109 Y MeSH Alpha-ketobutyric+acid PubChem CID 58 UNII B92RB6HY1A Y CompTox Dashboard (EPA) DTXSID9060524 InChI InChI=1S/C4H6O3/c1-2-3(5)4(6)7/h2H2,1H3,(H,6,7) YKey: TYEYBOSBBBHJIV-UHFFFAOYSA-N YInChI=1/C4H6O3/c1-2-3(5)4(6)7/h2H2,1H3,(H,6,7)Key: TYEYBOSBBBHJIV-UHFFFAOYAT SMILES O=C(C(=O)O)CC Properties Chemical formula C4H6O3 Molar mass 102.089 g/mol Appearance colorless solid Melting point 33 °C (91 °F; 306 K) Except where otherwise noted, data are given for materials in their standard state (at 25 °C [77 °F], 100 kPa). Y verify (what is YN ?) Infobox references Chemical compound α-Ketobutyric acid is an organic compound with the formula CH3CH2C(O)CO2H. It is a colorless solid that melts just above room temperature. Its conjugate base α-ketobutyrate is the predominant form found in nature (near neutral pH). It results from the lysis of cystathionine. It is also one of the degradation products of threonine, produced by the catabolism of the amino acid by threonine dehydratase. It is also produced by the degradation of homocysteine and the metabolism of methionine. α-Ketobutyrate is transported into the mitochondrial matrix, where it is converted to propionyl-CoA by branched-chain alpha-keto acid dehydrogenase complex. Further mitochondrial reactions produce succinyl-CoA. This is first through the enzyme mitochondria propionyl-CoA carboxylase with biotin as a cofactor to produce (S)-methylmalonyl-CoA. This is subsequently converted to (R)-methylmalonyl-CoA by mitochondrial methylmalonyl-CoA epimerase. Finally, mitochondrial methylmalonyl-CoA mutase with cofactor adenosylcobalamin produces succinyl-CoA which enters the citric acid cycle.[1] Conversion in sotonol in French vin jaune Vin jaune is marked by the formation of sotonol from alpha-ketobutyric acid.[2][3] See also Butyric acid α-Aminobutyric acid (homalanine) 2-Hydroxybutyric acid (α-hydroxybutyric acid) Other oxobutanoic acids 3-Oxobutanoic acid (acetoacetic acid) 4-Oxobutanoic acid (succinic semialdehyde) References ^ not specific enough to verify] ^ Pham TT, Guichard E, Schlich P, Charpenier C (1995). "Optimal Conditions for the Formation of Sotonol from α-Ketobutyric Acid in the French 'Vin Jaune'". *Journal of Agricultural and Food Chemistry*. 43 (10): 2616-2619. doi:10.1021/jf00058a012. ^ Guichard E, Pham TT, Etievant P (1993). "Quantitative Determination of Sotonol in Wines by High-Performance Liquid Chromatography". *Chromatographia*. 37 (9-10): 539-542. doi:10.1007/BF02275793. S2CID 95494741. Retrieved from " 3 Acetoacetic acid Names Preferred IUPAC name 3-Oxobutanoic acid[1] Systematic IUPAC name 3-Oxobutyric acid Other names Acetoacetic acidDiacetic acidAcetylacetic acidAcetonecarboxylic acid Identifiers CAS Number 541-50-4 Y 3D model (JSmol) Interactive image ChEBI CHEBI:15344 Y ChEMBL ChEMBL1230762 N ChemSpider 94 Y DrugBank DB01762 N KEGG C00164 Y PubChem CID 96 UNII 4ZI204Y1MC Y CompTox Dashboard (EPA) DTXSID00202441 InChI InChI=1S/C4H6O3/c1-3(5)2-4(6)7/h2H2,1H3,(H,6,7) YKey: WDJHALXBUFZDSR-UHFFFAOYSA-N YInChI=1/C4H6O3/c1-3(5)2-4(6)7/h2H2,1H3,(H,6,7)Key: WDJHALXBUFZDSR-UHFFFAOYAH SMILES O=C(C)CC(=O)O Properties Chemical formula C4H6O3 Molar mass 102.089 g·mol−1 Appearance Colorless, oily liquid Melting point 36.5 °C (97.7 °F; 309.6 K) Boiling point Decomposes Solubility in water Soluble Solubility in organic solvents Soluble in ethanol, ether Acidity (pKa) 3.58 [2] Except where otherwise noted, data are given for materials in their standard state (at 25 °C [77 °F], 100 kPa). N verify (what is YN ?) Infobox references Chemical compound Acetoacetic acid (IUPAC name: 3-Oxobutanoic acid, also known as Acetonecarboxylic acid or Diacetic acid) is the organic compound with the formula CH3COCH2COOH. It is the simplest beta-keto acid, and like other members of this class, it is unstable. The methyl and ethyl esters, which are quite stable, are produced on a large scale industrially as precursors to dyes. Acetoacetic acid is a weak acid.[3] Biochemistry Under typical physiological conditions, acetoacetic acid exists as its conjugate base, acetoacetate: AcCH2CO2H → AcCH2CO−2 + H+ Unbound acetoacetate is primarily produced by liver mitochondria from its thioester with coenzyme A (CoA): AcCH2C(O)−CoA + OH− → AcCH2CO−2 + H−CoA The acetoacetate-CoA itself is formed by three routes: 3-hydroxy-3-methylglutaryl CoA releases acetyl CoA and acetoacetate: −O2CCH2−C(Me)(OH)(−CH2C(O)−CoA → −O2CCH2−Ac + Ac−CoA Acetoacetyl-CoA can come from beta oxidation of butyryl-CoA: Et−CH2C(O)−CoA + 2NAD+ + H2O + FAD → Ac−CH2C(O)−CoA + 2NADH + FADH2 Condensation of pair of acetyl CoA molecules as catalyzed by thiolase.[4]:393 2Ac−CoA → AcCH2C(O)−CoA + H−CoA In mammals, acetoacetate produced in the liver (along with the other two "ketone bodies") is released into the bloodstream as an energy source during periods of fasting, exercise, or as a result of type 1 diabetes mellitus.[5] First, a CoA group is enzymatically transferred to it from succinyl CoA, converting it back to acetoacetyl CoA; this is then broken into two acetyl CoA molecules by thiolase, and these then enter the citric acid cycle. Heart muscle and renal cortex prefer acetoacetate over glucose. The brain uses acetoacetate when glucose levels are low due to fasting or diabetes.[4]:394 Synthesis and properties Acetoacetic acid may be prepared by the hydrolysis of diketene. Its esters are produced analogously via the reaction between diketene and alcohols.[3] and acetoacetic acid can be prepared by the hydrolysis of these species.[6] In general, acetoacetic acid is generated at 0 °C and used in situ immediately.[7] It decomposes at a moderate rate to acetone and carbon dioxide: CH3C(O)CH2CO2H → CH3C(O)CH3 + CO2 The acid form has a half-life of 140 minutes at 37 °C in water, whereas the basic form (the anion) has a half-life of 130 hours. That is, it reacts about 55 times more slowly.[8] The corresponding decarboxylation of trifluoroacetoacetate is used to prepare trifluoroacetone: CF3C(O)CH2CO2H → CF3C(O)CH3 + CO2 It is a weak acid (like most alkyl carboxylic acids), with a pKa of 3.58. Acetoacetic acid displays keto-enol tautomerisation, with the enol form being partially stabilised by extended conjugation and intramolecular H-bonding. The equilibrium is strongly solvent depended; with the keto form dominating in polar solvents (98% in water) and the enol form accounting for 25-49% of material in non-polar solvents.[9] Applications Pigment Yellow 16 is a typical dye containing the acetoacetyl group Acetoacetic esters are used for the acetoacetylation reaction, which is widely used in the production of arylide yellows and diarylide dyes.[3] Although the esters can be used in this reaction, diketene also reacts with alcohols and amines to the corresponding acetoacetic acid derivatives in a process called acetoacetylation. An example is the reaction with 4-aminoindane:[10] Detection Acetoacetic acid is measured in the urine of people with diabetes to test for ketoacidosis[11] and for monitoring people on a ketogenic or low-carbohydrate diet.[12][13] This is done using dipsticks coated in nitroprusside or similar reagents. Nitroprusside changes from pink to purple in the presence of acetoacetate, the conjugate base of acetoacetic acid, and the colour change is graded by eye. The test does not measure β-hydroxybutyrate, the most abundant ketone in the body; during treatment of ketoacidosis β-hydroxybutyrate is converted to acetoacetate so the test is not useful after treatment begins[11] and may be falsely low at diagnosis.[14] Similar tests are used in dairy cows to test for ketosis.[15] See also 3-Hydroxybutyrate dehydrogenase References ^ "Front Matter". *Nomenclature of Organic Chemistry : IUPAC Recommendations and Preferred Names 2013* (Blue Book). Cambridge: The Royal Society of Chemistry. 2014. p. 748. doi:10.1039/9781849733069-PP001. ISBN 978-0-85404-182-4. ^ Dawson, R. M. C., et al., Data for Biochemical Research, Oxford, Clarendon Press, 1959. ^ a b c Franz Dietrich Klingler; Wolfgang Ebertz (2005). "Oxocarboxylic Acids". *Ullmann's Encyclopedia of Industrial Chemistry*. Weinheim: Wiley-VCH. doi:10.1002/14356007.a18_313. ISBN 978-3527306732. ^ a b Lubert Stryer (1981). *Biochemistry* (2nd ed.). ^ Stryer, Lubert (1995). *Biochemistry* (Fourth ed.). New York: W.H. Freeman and Company. pp. 510–515, 581–613, 775–778. ISBN 0 7167 2009 4. ^ Robert C. Krueger (1952). "Crystalline Acetoacetic Acid". *Journal of the American Chemical Society*. 74 (21): 5536. doi:10.1021/ja01141a521. ^ Reynolds, George A.; VanAllan, J. A. (1952). "Methylglyoxal-*o*-Phenylhydrazone". *Organic Syntheses*. 32: 84. doi:10.15227/orgsyn.032.0084.; Collective Volume, vol. 4, p. 633 ^ Hay, R. W.; Bond, M. A. (1967). "Kinetics of decarboxilation of acetoacetic acid". *Aust. J. Chem.* 20 (9): 1823-8. doi:10.1071/CH9671823. ^ Grande, Karen D.; Rosenfeld, Stuart M. (1980). "Tautomeric equilibriums in acetoacetic acid". *The Journal of Organic Chemistry*. 45 (9): 1626-1628. doi:10.1021/jo01297a017. ISSN 0022-3263. ^ Kiran Kumar Solingapuram Sai; Thomas M. Gilbert; Douglas A. Klumpp (2007). "Knorr Cyclizations and Distonic Superelectrophiles". *J. Org. Chem.* 72 (25): 9761-9764. doi:10.1021/jo7013092. PMID 17999519. ^ a b Nyenwe, EA, Kitabchi, AE (April 2016). "The evolution of diabetic ketoacidosis: An update of its etiology, pathogenesis and management". *Metabolism: Clinical and Experimental*. 65 (4): 507-21. doi:10.1016/j.metabol.2015.12.007. PMID 26975543. ^ Hartman, AL; Vining, EP (January 2007). "Clinical aspects of the ketogenic diet". *Epilepsia*. 48 (1): 31-42. doi:10.1111/j.1528-1167.2007.00914.x. PMID 17241206. ^ Sumithran, Priya; Proietto, Joseph (2008). "Ketogenic diets for weight loss: A review of their principles, safety and efficacy". *Obesity Research & Clinical Practice*. 2 (1): 1-11. doi:10.1016/j.orcp.2007.11.003. PMID 24351673. ^ Misra, S; Oliver, NS (28 October 2015). "Diabetic ketoacidosis in adults" (PDF). *BMJ (Clinical Research Ed.)*. 351: h5660. doi:10.1136/bmj.h5660. hdl:10044/1/41091. PMID 26510442. ^ Tatone, EH; Gordon, JL; Hubbs, J; LeBlanc, SJ; DeVries, TJ; Duffield, TF (1 August 2016). "A systematic review and meta-analysis of the diagnostic accuracy of point-of-care tests for the detection of hyperketonemia in dairy cows". *Preventive Veterinary Medicine*. 130: 18-32. doi:10.1016/j.prevetmed.2016.06.002. PMID 27435643. Retrieved from " Butanedioic acid, polymer with 1,4-butanediol(C4H10O2.C4H6O4)x Discover more in SciFindernButanedioic acid, polymer with 1,4-butanediol. CAS Common Chemistry. CAS, a division of the American Chemical Society, n.d. (retrieved 2023-11-12) (CAS RN: 25777-14-4). Licensed under the Attribution-Noncommercial 4.0 International License (CC BY-NC 4.0). InChI=1S/C4H6O4.C4H10O2/c5-3(6)1-2-4(7)8;5-3-1-2-4-6/h1-2H2,(H,5,6)(H,7,8);5-6H,1-4H2InChIKey=FOINETJTVSEXPE-UHFFFAOYSA-NSMILES(CCC(O)=O)C(O)=O.C(COCOCOC)Canonical SMILESO=C(C)OCC(=O)O.O.CCCCOOther Names for this SubstanceButanedioic acid, polymer with 1,4-butanediolSuccinic acid, polyester with 1,4-butanediol1,4-Butanediol, polyester with succinic acid1,4-Butanediol, polymer with butanedioic acidPoly(tetramethylene succinate)Deleted or Replaced CAS Registry Numbers1783801-88-6