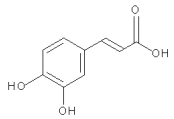

Formula: C9H8O4

MW: 180.16

CAS: 331-39-5

MDL: MFCD00004392

TNP: TNP00311

RARECHEM BK HC T335; TIMTEC-BB SBB006475; (2E)-3-(3,4-Dihydroxyphenyl)-2-propenoic acid; 2-Propenoic acid, 3-(3,4-dihydroxyphenyl)-; 3-(3,4-dihydroxyphenyl)-2-propenoicaci; 3-(3,4-Dihydroxyphenyl)propenoic acid; 3,4-Dihydroxybenzeneacrylic acid; 3,4-dihydroxyben

LogP: 8.22

LogS: -6.32

Acceptors: 4

Donors: 3

Rotation Bonds: 5

Chiral Centers: 0

N+O: 4

LIPINSKY: 3

IUPAC: (2E)-3-(3,4-dihydroxyphenyl)prop-2-enoic acid

Smiles: C(/C=Cc1cc(O)c(cc1)O)(=O)O

Specification: Pharmaceutical Intermediates; Aromatic Cinnamic Acids, Esters and Derivatives; Cinnamic acid; Organic acids; Antioxidant; Biochemistry Caffeic acid Chemical Properties:

mp 211-213 C (dec.)(lit.) storage temp. Store at RT. solubility ethanol: 50 mg/mL form powder color yellow to tan Water Solubility soluble in hot water Merck 14,1635 BRN 2210883 Stability:Stable. Combustible. Incompatible with strong oxidizing agents, strong bases. CAS DataBase Reference331-39-5(CAS DataBase Reference) NIST Chemistry ReferenceCinnamic acid, 3,4-dihydroxy-(331-39-5) EPA Substance Registry System2-Propenoic acid, 3-(3,4-dihydroxyphenyl)-(331-39-5) Safety Information Hazard Codes Xn,Xi Risk Statements 36/37/38-40-63-68 Safety Statements 26-36/37/39-36 WGK Germany 3 RTECS GD8950000 Hazard Note Irritant HS Code 29182990 Hazardous Substances Data331-39-5(Hazardous Substances Data) Caffeic acid English Caffeic acid Usage And Synthesis Chemical Properties:

Light yellow to greenish-yellow powder UsageConstituent of plants, probably occurs in plants only in conjugated forms. General DescriptionYellow prisms or plates (from chloroform or ligroin) or pale yellow granules. Alkaline solutions turn from yellow to orange. Air & Water ReactionsInsoluble in water. Reactivity ProfileCaffeic acid is a carboxylic acid. Carboxylic acids donate hydrogen ions if a base is present to accept them. They react in this way with all bases, both organic (for example, the amines) and inorganic. Their reactions with bases, called "neutralizations", are accompanied by the evolution of substantial amounts of heat. Neutralization between an acid and a base produces water plus a salt. Insoluble carboxylic acids react rapidly with aqueous solutions containing a chemical base and dissolve as the neutralization generates a soluble salt. Carboxylic acids in aqueous solution and liquid or molten carboxylic acids can react with active metals to form gaseous hydrogen and a metal salt. Such reactions occur in principle for solid carboxylic acids as well, but are slow if the solid acid remains dry. Even "insoluble" carboxylic acids may absorb enough water from the air and dissolve sufficiently in Caffeic acid to corrode or dissolve iron, steel, and aluminum parts and containers. Carboxylic acids, like other acids, react with cyanide salts to generate gaseous hydrogen cyanide. The reaction is slower for dry, solid carboxylic acids. Insoluble carboxylic acids react with solutions of cyanides to cause the release of gaseous hydrogen cyanide. Flammable and/or toxic gases and heat are generated by the reaction of carboxylic acids with diazo compounds, dithiocarbamates, isocyanates, mercaptans, nitrides, and sulfides. Carboxylic acids, especially in aqueous solution, also react with sulfites, nitrites, thiosulfates (to give H2S and SO3), dithionites (SO2), to generate flammable and/or toxic gases and heat. Their reaction with carbonates and bicarbonates generates a harmless gas (carbon dioxide) but still heat. Like other organic compounds, carboxylic acids can be oxidized by strong oxidizing agents and reduced by strong reducing agents. These reactions generate heat. A wide variety of products is possible. Like other acids, carboxylic acids may initiate polymerization reactions; like other acids, they often catalyze (increase the rate of) chemical reactions. Health HazardACUTE/CHRONIC HAZARDS: When heated to decomposition Caffeic acid emits acrid smoke and fumes. Fire HazardFlash point data for Caffeic acid are not available; however, Caffeic acid is probably combustible. Caffeic acid

Merck 13 Reference: Monograph Number: 0001635

Title: Caffeic Acid

CAS Registry Number: 331-39-5

CAS Name: 3-(3,4-Dihydroxyphenyl)-2-propenoic acid

Additional Names: 3,4-dihydroxycinnamic acid

Molecular Formula: C9H8O4

Molecular Weight: 180.16.

Percent Composition: C 60.00%, H 4.48%, O 35.52%

Literature References: Constituent of plants, probably occurs in plants only in conjugated forms, e.g., chlorogenic acid. Isoln from green coffee: Wolfrom et al., J. Agric. Food Chem. 8, 58 (1960); from roasted coffee: Krasemann, Arch. Pharm. 293, 721 (1960). Formation by acid hydrolysis of chlorogenic acid: Fiedler, Arzneim.-Forsch. 4, 41 (1954); Whiting, Carr, Nature 180, 1479 (1957); Guern, C.A. 61, 9965h (1964). Synthesis: Hayduck, Ber. 36, 2935 (1903); Posner, J. Prakt. Chem. 82, 432 (1910); Mauthner, ibid. 142, 33 (1935); Pandya et al., Proc. Indian Acad. Sci. 9A, 511 (1939); Neish, Can. J. Biochem. Physiol. 37, 1431 (1959). Review: Herrmann, Pharmazie 11, 433 (1956).

Properties: Yellow crystals from concd aq solns. Monohydrate from dil solns. Dec 223-225 (softens at 194). Rf values: Fiedler, loc. cit. Sparingly sol in cold water. Freely sol in hot water, cold alc. Alkaline solns turn from yellow to orange.

Derivative Type: Methyl ester

Molecular Formula: C10H10O4

Molecular Weight: 194.18.

Percent Composition: C 61.85%, H 5.19%, O 32.96%

Properties: Colorless needles from water, mp 152-153.

Melting point: mp 152-153