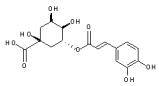

Formula: C16H18O9

MW: 354.31

CAS: 327-97-9

MDL: MFCD01104103

TNP: TNP00127

LogP: -3.29

LogS: -2.15

Acceptors: 9

Donors: 6

Rotation Bonds: 7

Chiral Centers: 4

N+O: 9

LIPINSKY: 3

IUPAC: 3-[(2E)-3-(3,4-dihydroxyphenyl)prop-2-enoyloxy](1S,3R,4R,5R)-1,4,5-trihydroxyc
yclohexanecarboxylic acid

Smiles: O(C(/C=Cc1cc(O)c(cc1)O)=O)[C@@H]1CC(C(=O)O)(O)CC(C1O)O

Merck 13 Reference: Monograph Number: 0002161

Title: Chlorogenic Acid

CAS Registry Number: 327-97-9

CAS Name:
[1S-(1a,3b,4a,5a)]-3-[[3-(3,4-Dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxycyclohexa
necarboxylic acid

Additional Names: 1,3,4,5-tetrahydroxycyclohexanecarboxylic acid 3-(3,4-dihydroxycinnamate);

3-caffeoylquinic acid; 3-(3,4-dihydroxycinnamoyl)quinic acid

Molecular Formula: C16H18O9

Molecular Weight: 354.31.

Percent Composition: C 54.24%, H 5.12%, O 40.64%

Literature References: Important factor in plant metabolism. Isoln from green coffee beans: Freudenberg, Ber. 53, 237 (1920). Chlorogenic acid and its isomers isochlorogenic acid and neochlorogenic acid occur also in fruit, leaves and other tissues of dicotyledenous plants: Sondheimer, Arch. Pharm. 293, 721 (1960). Forms caffeic acid on hydrolysis: Fiedler, Arzneim.-Forsch. 4, 41 (1954). Structure: Fischer, Dangschat, Ber. 65, 1037 (1932); Barnes et al., J. Am. Chem. Soc. 72, 4178 (1950); Corse et al., Tetrahedron 18, 1207 (1962). Synthesis: Panizzi et al., Gazz. Chim. Ital. 86, 913 (1956).

Derivative Type: Hemihydrate

Properties: Needles from water. Becomes anhydr at 110. mp 208. [a]D26 -35.2 (c = 2.8). pKa (27) 2.66. Rf values: Fiedler, loc. cit. Soly in water at 25 about 4%, much more sol in hot water. Alkaline solns acquire an orange color. Freely sol in alcohol, acetone. Very slightly sol in ethyl acetate. Heating with dil HCl yields caffeic acid. Forms a black compd with iron, said to be responsible for the blackening of cut and cooked potatoes: Chem. Ind. (London) 1958, 627.

Melting point: mp 208

pKa: pKa (27) 2.66

Optical Rotation: [a]D26 -35.2 (c = 2.8)

Derivative Type: 3