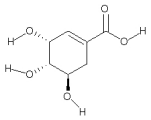

Formula: C7H10O5

MW: 174.15

CAS: 138-59-0

MDL: MFCD00069511

TNP: TNP00387

LogP: -3.07

LogS: -1.35

Acceptors: 5

Donors: 4

Rotation Bonds: 2

Chiral Centers: 3

N+O: 5

LIPINSKY: 4

Info: Isoln from fruit of plant Illicium religiosum Sieb.

IUPAC: (4S,3R,5R)-3,4,5-trihydroxycyclohex-1-enecarboxylic acid

Smiles: C1[C@H]([C@H](O)[C@@H](C=C1C(O)=O)O)O

Merck 13 Reference: Monograph Number: 0008555

Title: Shikimic Acid

CAS Registry Number: 138-59-0

CAS Name: [3R-(3a,4a,5b)]-3,4,5-Trihydroxy-1-cyclohexene-1-carboxylic acid

Molecular Formula: C7H10O5

Molecular Weight: 174.15.

Percent Composition: C 48.28%, H 5.79%, O 45.94%

Literature References: Naturally occurring (-)-form is a major biosynthetic precursor of phenylalanine, tyrosine, and tryptophan and hence of the majority of plant alkaloids. It is also involved in the biosynthesis of lignin, q.v., flavonoids and other important aromatic compounds. Isoln from the fruit of the oriental plant Illicium religiosum Sieb. et Zucc., Magnoliaceae (called in Japanese shikimi-no-ki): J. F. Eykman, Rec. Trav. Chim. 4, 32 (1885); idem, Ber. 24, 1278 (1891). Structural study: H. O. L. Fischer, G. Dangshat, Helv. Chim. Acta 17, 1200 (1934). Configuration: eidem, ibid. 18, 1206 (1935); 20, 705 (1937). Conformation in soln: L. D. Hall, J. Org. Chem. 29, 297 (1964). Enzymatic synthesis: P. R. Srinivasan et al., J. Am. Chem. Soc. 77, 4943 (1955). Stereospecific synthesis: R. McCrindle et al., J. Chem. Soc. 1960, 1560; E. E. Smissman et al., J. Am. Chem. Soc. 84, 1040 (1962). Improved synthesis: J. L. Pawlak, G. A. Berchtold, J. Org. Chem. 52, 1765 (1987). Synthesis of the (