



Formula: C₁₁H₁₄O₅

MW: 226.23

CAS: 6902-77-8

MDL:

TNP: TNP00646

cyclopenta(c)pyran-4-carboxylic acid, 1,4a- α ,5,7a- α -tetrahydro-1-hydroxy; GENIPIN; 1,4a,5,7a-tetrahydro-1-hydroxy-7-(hydroxymethyl)-cyclopenta(c)pyran-4-carboxylic acid methyl ester; Methyl (1S,2R,6S)-2-hydroxy-9-(hydroxymethyl)-3-oxabicyclo[4.3.0]nona-



LogP: 0.67

LogS: -2.95

Acceptors: 5

Donors: 2

Rotation Bonds: 4

Chiral Centers: 3

N+O: 5

LIPINSKY: 4

IUPAC: methyl (4aS,7aS,1R)-1-hydroxy-7-(hydroxymethyl)-1,5,4a,7a-tetrahydro-4aH-cyclopenta[1,2-d]pyran-4-carboxylate

Smiles: C(C1=CC[C@@H]2(C(=CO[C@H]([C@H]12)O)C(OC)=O))O

SOURCE: Genipin is an aglycone derived from geniposide, which is found in the fruit of

Gardenia jasminoides Elli

ACTIVITY: Genipin is a hydrolytic product of geniposide, which is found in the fruit of *Gardenia jasminoides* Ellis. The components of the fruit have been used in traditional Chinese medicine and as a blue colorant by food industries in East Asia. The structure of genipin was discovered in the 1960