



Formula: C₁₅H₁₈O₈

MW: 326.3

CAS: 33570-04-6

MDL: MFCD06668131

TNP: TNP00251

BILOBALID; (-)-BILOBALIDE; BILOBALIDE;
5,3'-DIHYDROXY-3,6,7,4'-TETRAMETHOXYFLAVONE;
4H,5AH,9H-FURO[2,3-B]FURO[3',2':2,3]CYCLOPENTA[1,2-C]FURAN-2,4,7(3H,8H)-TRIONE,9
-(1,1-DIMETHYLETHYL)-10,10A-DIHYDRO-8,9-DIHYDROXY-,
[5AR-(3AS*,5A,8,8AS*,9,10A)]-; 3',5-DIHYDROX



LogP: 3.32

LogS: -4.61

Acceptors: 8

Donors: 2

Rotation Bonds: 0

Chiral Centers: 6

N+O: 8

LIPINSKY: 4

IUPAC: (1S,8S,12S,5R,14R)-14-(tert-butyl)-2,14-dihydroxy-4,6,11-trioxatetracyclo[6.6.0.0.0]tetradecane-3,7,10-trione

Smiles:

C1([C@@]23[C@]4([C@@](C[C@@H]2(OC(C3)=O))(C(C)(C)C)O)[C@H](O1)(OC([C@@H]4O)=O))=O

REFERENCE: # ^ van Beek TA, Montoro P (2009). "Chemical analysis and quality control of Ginkgo biloba leaves, extracts, and phytopharmaceuticals". Journal of Chromatography A 1216 (11): 2002