



Formula: C<sub>20</sub>H<sub>30</sub>O<sub>5</sub>

MW: 350.46

CAS: 5508-58-7

MDL: MFCD01103302

TNP: TNP00114

ANDRO; ANDROGRAPHIS; ANDROGRAPHOLIDE;  
3A,14,15,18-TETRAHYDROXY-5B,9B,H,10A-LAMBDA-8,20-DIENE;  
2(3H)-FURANONE,3-[2-[(1R,4AS,5R,6R,8AS)-DECAHYDRO-6-HYDROXY-5-(HYDROXYMETHYL)-5,8A-DIMETHYL-2-METHYLENE-1-NAPHTHALENYL]ETHYLIDENE]DIHYDRO-4-HYDROXY-, (3E,4S)-; 2(3h)-



LogP: 5.06

LogS: -5.27

Acceptors: 5

Donors: 3

Rotation Bonds: 6

Chiral Centers: 6

N+O: 5

LIPINSKY: 4

IUPAC: 4-hydroxy-3-{2-[8-hydroxy-7-(hydroxymethyl)-1,7-dimethyl-3-methylenebicyclo[4.4.0]dec-2-yl]ethylidene}-4,5-dihydrofuran-2-one

Smiles: CC12C(C(CO)(C)C(CC2)O)CCC(C1CC=C1C(O)COC1=O)=C

Specification: Di-Terpenoids; Asymmetric Synthesis; Chiral Building Blocks; Complex Molecules  
Andrographolide Chemical Properties:

mp 229-232 C(lit.) alpha -126