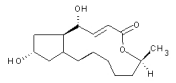

Formula: C16H24O4

MW: 280.36

CAS: 20350-15-6

TNP NUMBER: TNP00146

MDL NUMBER: MFCD05618218

IUPAC: (7S,15S,1R)-2,15-dihydroxy-7-methyl-6-oxabicyclo[11.3.0]hexadeca-3,11-dien-5-o ne

Smiles: C1[C@H](CC2[C@@H]1[C@@H](C=CC(=O)O[C@H](CCCC=C2)C)O)O

REFERENCE: Reference Dinter, A. and Berger, E.G., Golgi-disturbing agents. Histochem. Cell Biol. 109, 571-590, (1998) abstract Shao, R.G., et al., Brefeldin A is a potent inducer of apoptosis in human cancer cells independently of p53. Exp. Cell Res. 227, 190-196, (1996) abstract Guo, H., et al., Brefeldin A-mediated apoptosis requires the activation of capases and is inhibited by Bcl-2. Exp. Cell Res. 245, 57-68, (1998) abstract Linardic, C.M., et al., Activation of the sphingomyelin cycle by brefeldin A: effects of brefeldin A on differentiation and implications for a role for ceramide in regulation of protein trafficking. Cell. Growth Differ. 7, 765-774, (1996) abstract Merck Merck 13,1355 Beilstein Beil. 18,IV,1220

SOURCE: from Penicillium brefeldianum,

ACCEPTORS: 4

DONORS: 2

ROTATION BONDS: 0

N+O: 4

Chiral Centers: 5

LogP: 3.15

LogS: -4.12

LIPINSKI: 4

Monograph Number: 0001355

Title: Brefeldin A

CAS Registry Number: 20350-15-6

CAS Name:
1,6,7,8,9,11a,12,13,14,14a-Decahydro-1,13-dihydroxy-6-methyl-4H-cyclopent[f]oxacyclotridecin-4-one

Additional Names: g,4-dihydroxy-2-(6-hydroxy-1-heptenyl)-4-cyclopentanecrotonic acid l-lactone; ascotoxin; cyanein; decumbin

Molecular Formula: C16H24O4

Molecular Weight: 280.36.

Percent Composition: C 68.54%, H 8.63%, O 22.83%

Literature References: A fungal metabolite which is a macrocyclic lactone exhibiting a wide range of antibiotic activity. Produced by Penicillium brefeldianum Dodge: E. Haerri et al., Helv. Chim. Acta 46, 1235 (1963). Also produced by P. decumbens: V. L. Singleton et al., Nature 181, 1072 (1958); P. cyaneum: V. Betina et al., Folia Microbiol. 7, 353 (1962). Structure: H. P. Sigg, Helv. Chim. Acta 47, 1401 (1964). Abs configuration: H. P. Weber et al., ibid. 54, 2763 (1971). Synthesis of (