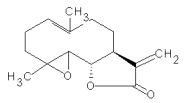

Formula: C15H20O3

MW: 248.32

CAS: 20554-84-1

TNP NUMBER: TNP00292

MDL NUMBER: MFCD06668140

IUPAC: (1S,11S)-4,8-dimethyl-12-methylene-3,14-dioxatricyclo[9.3.0.0]tetradec-7- en-13-one

Smiles: O1C2[C@H]3OC(=O)C([C@@H]3CCC(=CCCC12C)C)=C

isolation from chrisanthemum parthenium

REFERENCE: Kwok, B.H., et al., The anti-inflammatory natural product parthenolide from the medicinal herb Feverfew directly binds to and inhibits I?B kinase. Chem. Biol. 8, 759-766, (2001) Pozarowski, P., et al., NF-?B inhibitor sesquiterpene parthenolide induces concurrently atypical apoptosis and cell necrosis: difficulties in identification of dead cells in such cultures. Cytometry 54A, 118-124, (2003) Garcia-Pineres, A.J., et al., Cysteine 38 in p65/NF-?B plays a crucial role in DNA binding inhibition by sesquiterpene lactones. J. Biol. Chem. 276, 39713-39720, (2001) Wen, J., et al., Oxidative stress-mediated apoptosis. The anticancer effect of the sesquiterpene lactone parthenolide. J. Biol. Chem. 277, 38954-38964, (2002) Merck Merck 13,7120 Beilstein Beil. 19,IV,1731 reference RegBook 1 (1), 809:E / Structure Index 1, 126:A:8

SOURCE: isolation from chrisanthemum parthenium

ACCEPTORS: 3

DONORS: 0

ROTATION BONDS: 0

N+O: 3

Chiral Centers: 4

LogP: 4.54

LogS: -4.5

LIPINSKI: 4

Monograph Number: 0007120

Title: Parthenolide

CAS Registry Number: 20554-84-1

CAS Name:
(1aR,4E,7aS,10aS,10bS)-2,3,6,7,7a,8,10a,10b-Octahydro-1a,5-dimethyl-8-methyleneoxireno[9,10]cyclodeca[1,2-b]furan-9(1aH)-one

Additional Names: 4,5a-epoxy-6b-hydroxy-germacra-1(10),11(13)-dien-12-oic acid g-lactone

Molecular Formula: C15H20O3

Molecular Weight: 248.32.

Percent Composition: C 72.55%, H 8.12%, O 19.33%

Literature References: Sesquiterpene lactone found in feverfew, q.v., and in other plants. Isolation from Chrysanthemum parthenium (L.) Bernh. Compositae and characterization: V. Herout et al., Chem. Ind. (London) 1959, 1069; M. Soucek et al., Collect. Czech. Chem. Commun. 26, 803 (1961); from Magnolia grandiflora L., Magnoliaceae: F. S. El-Feraly, Y.-M. Chan, J. Pharm. Sci. 67, 347 (1978). Revised structure and spectral analysis: T. R. Govindachari et al., Tetrahedron 21, 1509 (1965). Absolute configuration: A. S. Bawdekar et al., Tetrahedron Lett. 1966, 1225. Crystal structure: A. Quick, D. Rogers, J. Chem. Soc. Perkin Trans. 2 4, 465 (1976). HPLC determn: D. Strack et al., Z. Naturforsch. 35, 915 (1980). Cytotoxicity: K.-H. Lee et al., Cancer Res. 31, 1649 (1971); L. A. J. O'Neill et al., Br. J. Clin. Pharmacol. 23, 81 (1987).

Properties: Colorless plates, mp 115-116. [a]D20 -81.4 (c = 1.04 in chloroform); [a]D22 -71.4 (c = 0.220 in CH2Cl2). uv max: 214 nm (log e 4.22).

Melting point: mp 115-116

Optical Rotation: [a]D20 -81.4 (c = 1.04 in chloroform); [a]D22 -71.4 (c = 0.220 in CH2Cl2)

Absorption maximum: uv max: 214 nm (log e 4.22)