



Formula: C₃₀H₄₆O₄

MW: 470.69

CAS: 471-53-4

TNP NUMBER: TNP00130

MDL NUMBER: MFCD00599051

IUPAC: (5S,8S,15S,18S,1R,2R,10R,14R,20R)-18-hydroxy-1,2,5,8,15,19,19-heptamethyl-13-oxopentacyclo[12.8.0.0.0.0]docos-11-ene-8-carboxylic acid

Smiles:

C=12[C]([C]3(CC[C@@H]4([C]([C@H]3(C(C1)=O)))(CC[C@@H](O)C4(C)C))C)(CC[C]1([C@H]2(C[C@@](C(=O)O)(CC1)C))C)C

THERAPEUTIC CATEGORY: Anti-inflammatory (Topical)

SOURCE: Preparation From licorice root. Made from glycyrrhizic acid from *Glycyrrhiza glabra* L., Leguminosae

ACCEPTORS: 4

DONORS: 2

ROTATION BONDS: 1

N+O: 4

Chiral Centers: 9

LogP: 9.53

LogS: -7.01

LIPINSKI: 3

