



Formula: C₂₄H₄₀O₅

MW: 408.58

TNP NUMBER: TNP00437

MDL NUMBER: MFCD02940838

IUPAC: 4-((1S,2S,7S,11S,16S,5R,9R,10R,14R,15R)-5,9,16-trihydroxy-2,15-dimethyltetracyclo[8.7.0.0.0<2,7>.0<11,15>]heptadec-14-yl)pentanoic acid

Smiles:

C1[C@@H](CC[C@H]2([C@@H]1(C[C@H]([C@@H]1([C@@H]2(C[C@@H]([C]2([C@H]1(CC[C@@H]2([C@H](C)CCC(O)=O)))C(O)))O))C)O

Cholic acid 97%, occurs in biles of most vertebrates

THERAPEUTIC CATEGORY: Choleric

ACCEPTORS: 5

DONORS: 4

ROTATION BONDS: 4

N+O: 5

Chiral Centers: 11

LogP: 5.68

LogS: -5.35

LIPINSKI: 4

