



Formula: C₂₀H₂₄O₁₀

MW: 424.4

CAS: 15291-77-7

MDL: MFCD06668132

TNP: TNP00253

B,B-DIMETHYLACRYLALKANNIN



LogP: 1.31

LogS: -2.89

Acceptors: 10

Donors: 3

Rotation Bonds: 0

Chiral Centers: 11

N+O: 10

LIPINSKY: 4

IUPAC: (7S,8S,13S,16S,1R,3R,10R,11R,17R)-8-(tert-butyl)-6,12,17-trihydroxy-16-methyl-2,4,14,19-tetraoxahexacyclo[8.7.2.0.0.0.0]nonadecane-5,15,18-trione

Smiles:

O1[C@@H]2([C]([C@@H](C1=O)C)([C@@]13[C@@]4([C@@H]2O)[C@@]2([C@H](O1)(OC([C@@H]2O)=O))C(C[C@H]4OC3=O)[C@@](C)(C)C)O

SOURCE: Ginkgolide B from Ginkgo biloba leaves

Specification: B,B-DIMETHYLACRYLALKANNIN

B,B-DIMETHYLACRYLALKANNIN Usage And Synthesis B,B-DIMETHYLACRYLALKANNIN