



Formula: C₁₅H₁₆O₆

MW: 292.29

CAS: 17617-45-7

TNP NUMBER: TNP00135

MDL NUMBER: MFCD02114017

IUPAC: (5S,8S,12S,1R,3R,9R,13R,14R)-1-hydroxy-13-methyl-14-(1-methylvinyl)-4,7,10-trioxapentacyclo[6.4.1.1.0.0]tetradecane-6,11-dione

Smiles:

O1[C@@]23[C]4([C@@]([C@H]5C(=O)O[C@@H]([C@H]4OC3=O)[C@H]5C(=C)C)(O)C[C@@H]12)C

Active Component of Picrotoxin. Picrotoxin isolated from from the seeds of Anamirta Cocculus

THERAPEUTIC CATEGORY: CNS and respiratory stimulant

ACCEPTORS: 6

DONORS: 1

ROTATION BONDS: 0

N+O: 6

Chiral Centers: 8

LogP: 1.97

LogS: -3.69

LIPINSKI: 4

Synonyms:

6a-beta,8as*,8b-beta,9r*)-6-beta;ahydro-2a-hydroxy-8b-methyl-9-(1-methylethenyl)-,(1ar-(1a-al pha,2a-beta,3-bet;PICROTOXININ

CAS:17617-45-7

MF:C15H16O6

MW:292.28

EINECS:

Product Categories:Miscellaneous Natural Products;AntagonistsIon Channels;GABA and Glycine Receptor Modulators;GABAergics;Ligand-Gated Ion Channels;Neurotransmitters
PICROTOXININ

Chemical Properties: mp 203-205C T+ Risk Statements 25-28 Safety Statements
13-20-45-36/37-28 RIDADR 3172 RTECS PC5150000 HazardClass 6.1(a) PackingGroup I
PICROTOXININ

Usage And Synthesis: PICROTOXININ

