



Formula: C₂₂H₂₂O₈

MW: 414.41

CAS: 518-28-5

MDL: MFCD00601260

TNP: TNP00237

5,8,8a,9-tetrahydro-9-hydroxy-5-(3,4,5-trimethoxyphenyl)-furo(3',4':6,7)naphtho(2,3-d)-1,3-dioxol-6(5ah)-one;
(5R,5AR,8AR,9R)-9-HYDROXY-5-(3,4,5-TRIMETHOXY-PHENYL)-5,8,8A,9-TETRAHYDRO-5A
H-FURO[3',4':6,7]NAPHTHO[2,3-D][1,3]DIOXOL-6-ONE; 4,5-trimethoxyphenyl



LogP: 3.21

LogS: -4.62

Acceptors: 8

Donors: 1

Rotation Bonds: 2

Chiral Centers: 4

N+O: 8

LIPINSKY: 4

Info: Podophyllotoxin 95%

IUPAC: (5R,9R,5aR,8aR)-9-hydroxy-5-(3,4,5-trimethoxyphenyl)-5,8,9,5a,8a-pentahydro-2H
-isobenzofurano[5',6'-2,1]benzo[4,5-d]1,3-dioxolan-6-one

Smiles:

O=C1OC2C(OC)OC3C(OC)OC(OC)C3OC2C1

Specification: Plant Oils, Toxins, Phenolic Acids & Derivatives; Natural Plant Extract; Microtubule Inhibitors Cancer Research; Microtubule Inhibitors; Antitumor Agents; Cell Signaling and Neuroscience; Cytoskeleton and Extracellular Matrix

(5R,5aR,8aR,9R)-5,8,8a,9-Tetrahydro-9-hydroxy-5-(3,4,5-trimethoxyphenyl)-furo(3',4':6,7)naptho[2,3-d]-1,3-dioxol-6(5aH)-one Chemical Properties:

mp 183-184 C(lit.) alpha -110.7