



Formula: C₂₂H₂₃NO₇

MW: 413.43

CAS: 128-62-1

MDL: MFCD01109038

TNP: TNP00034

,2,3,4-tetrahydroisoquinaline;
[S-(R*,S*)]-6,7-Dimethoxy-3-(5,6,7,8-tetrahydro-4-methoxy-6-methyl-1,3-dioxolo[4,5-g]isoquinolin-5-yl)-1(3H)-isobenzofuranone; 1(3H)-Isobenzofuranone,
6,7-dimethoxy-3-(5,6,7,8-tetrahydro-4-methoxy-6-methyl-1,3-dioxolo[4,5-g]is



LogP: -3.97

LogS: -2.92

Acceptors: 7

Donors: 0

Rotation Bonds: 4

Chiral Centers: 2

N+O: 8

LIPINSKY: 4

IUPAC: (3R)-3-((5R)-4-methoxy-6-methyl(5,6,7,8-tetrahydro-2H-1,3-dioxoleno[4,5-g]isoquinolin-5-yl))-6,7-dimethoxy-3-hydroisobenzofuran-1-one

Smiles: c12C(O[C@H](c1ccc(c2OC)OC)([C@H]1(c2c(c3OCOC3cc2CCN1C)OC)))=O

THERAPEUTIC CATEGORY: Antitussive

REFERENCE: Merk, 12th Ed., 6815

Specification: Intermediates & Fine Chemicals; Pharmaceuticals; Asymmetric Synthesis; Chiral Building Blocks; Complex Molecules Narcotine Chemical Properties:

mp 174-176 C(lit.) alpha -200