



Formula: C₂₁H₂₁NO₆

MW: 383.4

CAS: 118-08-1

TNP NUMBER: TNP00262

MDL NUMBER: MFCD00599507

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

Smiles: c12C(O[C@@H](c1ccc(c2OC)OC)([C@H]1(c2c(cc3c(c2)OCO3)CCN1C)))=O

naturally occurring L-beta form from *Hydrastis canadensis* L., Ranunculaceae together with berberine and canadine

THERAPEUTIC CATEGORY: hydrochloride formerly as uterine hemostatic, antiseptic

ACCEPTORS: 6

DONORS: 0

ROTATION BONDS: 3

N+O: 7

Chiral Centers: 2

LogP: 3.2

LogS: -4.63

LIPINSKI: 4

Synonyms: HYDRASTINE;HYDRASTINE,
(-)-B-;(-)-BETA-HYDRASTINE;(-)-B-HYDIASTINE;(1R,9S)-(-)-BETA-HYDRASTINE;(1R,9S)-BE
TA-HYDRASTINE;[S-(R*,S*)]-6,7-Dimethoxy-3-(5,6,7,8-tetrahydro-6-methyl-1,3-dioxolo[4,5-g]is
oquinolin-5-yl)-1(3H)-isobenzofuranone;1(3H)-Isobenzofuranone,
6,7-dimethoxy-3-(5,6,7,8-tetrahydro-6-methyl-1,3-dioxolo[4,5-g]isoquinolin-5-yl)-, [S-(R*,S*)]-

CAS:118-08-1

MF:C21H21NO6

MW:383.39

EINECS:204-233-0

Product Categories: (-)-BETA-HYDRASTINE

Chemical Properties: storage temp. -20C

CAS DataBase Reference: 118-08-1(

CAS DataBase Reference:) Xn Risk Statements 20/21/22 Safety Statements 36 RIDADR 1544
WGK Germany 3 RTECS MU6030000 HazardClass 6.1(b) PackingGroup III
(-)-BETA-HYDRASTINE

Usage And Synthesis: (-)-BETA-HYDRASTINE

