Hydrastine

Other names: 1(3H)-Isobenzofuranone, 6,7-dimethoxy-3-(5,6,7,8-tetrahydro-6-methyl-1,3-dioxolo[4,5-g]isoquinolin-5-yl)-
6,7-Dimethoxy-3-(6-methyl-5,6,7,8-tetrahydro[1,3]dioxolo[4,5-g]isoquinolin-5-yl)-2-benzof
Phthalide, 6,7-dimethoxy-3-(5,6,7,8-tetrahydro-6-methyl-1,3-dioxolo(4,5-g)isoquinolin-5-yl)-
[S-(R*,S*)]-6,7-Dimethoxy-3-(5,6,7,8-tetrahydro-6-methyl-1,3-dioxolo[4,5-g]isoquinolin-5-y
l-«beta»-Hydrastine
l-Â«betaÂ»-Hydrastine

Inchi: InChI=1S/C21H21NO6/c1-22-7-6-11-8-15-16(27-10-26-15)9-13(11)18(22)19-12-4-5-14(2

InchiKey: JZUTXVTYJDCMDU-UHFFFAOYSA-N

Formula: C21H21NO6

SMILES: COc1ccc2c(c1OC)C(=O)OC2C1c2cc3c(cc2CCN1C)OCO3

Mol. weight [g/mol]: 383.39

CAS: 118-08-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.11		Aqueous Solubility Prediction Method
logp	2.873		Crippen Method
mcvol	267.550	ml/mol	McGowan Method
rinpol	2985.00		NIST Webbook
rinpol	2988.00		NIST Webbook
tf	389.65	K	Aqueous Solubility Prediction Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C118081&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point