Hydrocotarnine

Other names: 1,3-Dioxolo[4,5-g]isoquinoline, 5,6,7,8-tetrahydro-4-methoxy-6-methyl-
Hydrocotarnin
4-Methoxy-6-methyl-5,6,7,8-tetrahydro-1,3-dioxolo(4,5-g)isoquinoline
Inchi: InChI=1S/C12H15NO3/c1-13-4-3-8-5-10-12(16-7-15-10)11(14-2)9(8)6-13/h5H,3-4,6-7H2
InchiKey: XXANNZJIZQTCBP-UHFFFAOYSA-N
Formula: C12H15NO3
SMILES: COc1c2c(cc3c1OCO3)CCN(C)C2
Mol. weight [g/mol]: 221.25
CAS: 550-10-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.37		Crippen Method
logp	1.412		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
rinpol	1790.00		NIST Webbook
rinpol	1798.00		NIST Webbook
rinpol	1790.00		NIST Webbook
rinpol	1798.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C550107&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices