Carnegine

Other names:	Isoquinoline, 1,2,3,4-tetrahydro-6,7-dimethoxy-1,2-dimethyl-, (.+/-.)- Carnegin Pectenin Pectenine Isoquinoline, 1,2,3,4-tetrahydro-6,7-dimethoxy-1,2-dimethyl-, (±)- (+/-)-Pectenine
Inchi:	InChI=1S/C13H19NO2/c1-9-11-8-13(16-4)12(15-3)7-10(11)5-6-14(9)2/h7-9H,5-6H2,1-4H
InchiKey:	HRSIPKSSEVRSPG-UHFFFAOYSA-N
Formula:	C13H19NO2
SMILES:	COc1cc2c(cc1OC)C(C)N(C)CC2
Mol. weight [g/mol]:	221.30
CAS:	490-53-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.66		Crippen Method
logp	2.253		Crippen Method
mcvol	181.130	ml/mol	McGowan Method
rinpol	1727.00		NIST Webbook
rinpol	1727.00		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=C490539&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