

Cacalohastine

Inchi: InChI=1S/C16H18O2/c1-9-6-5-7-12-13(9)11(3)14-10(2)8-18-16(14)15(12)17-4/h5,7-9H,6
InchiKey: WCJNJWNPAYBQPW-SECBINFHSA-N
Formula: C16H18O2
SMILES: COc1c2c(c(C)c3c(C)coc13)C(C)CC=C2
Mol. weight [g/mol]: 242.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.98		Crippen Method
logp	4.579		Crippen Method
mcvol	193.960	ml/mol	McGowan Method
rinpol	2055.00		NIST Webbook
rinpol	2055.00		NIST Webbook
ripol	2820.00		NIST Webbook
ripol	2820.00		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=R616092&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
ripol: Polar retention indices

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