

Dihydroisochromolaenin

Inchi: InChI=1S/C15H18O/c1-9-4-5-12-10(2)7-14-15(13(12)6-9)11(3)8-16-14/h4,6,8,10,12H,5,7
InchiKey: UEAPOVJEVUNJHK-NUHJPDEHSA-N
Formula: C15H18O
SMILES: CC1=CCC2C(=C1)c1c(C)coc1CC2C
Mol. weight [g/mol]: 214.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.98		Crippen Method
logp	4.130		Crippen Method
mcvol	178.300	ml/mol	McGowan Method
rinpol	1763.00		NIST Webbook
rinpol	1763.00		NIST Webbook
ripol	2373.00		NIST Webbook
ripol	2373.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R320984&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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