

1,6-Dihydrochromolaenin

Inchi:	InChI=1S/C15H18O/c1-9-4-5-12-10(2)7-14-15(13(12)6-9)11(3)8-16-14/h6,8,10,12H,1,4-5
InchiKey:	FWAMSVJFINPKEF-NUHJPDEHSA-N
Formula:	C15H18O
SMILES:	C=C1C=C2c3c(C)coc3CC(C)C2CC1
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
ripol	2383.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R321041&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.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
ripol:	Polar retention indices

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