

Chromolaenin

Inchi: InChI=1S/C15H16O/c1-9-4-5-12-10(2)7-14-15(13(12)6-9)11(3)8-16-14/h4-6,8,10H,7H2,1H
InchiKey: CTILMUMVHPOCNU-JTQLQIEISA-N
Formula: C15H16O
SMILES: Cc1ccc2c(c1)-c1c(C)coc1CC2C
Mol. weight [g/mol]: 212.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.81		Crippen Method
logp	4.223		Crippen Method
mcvol	174.000	ml/mol	McGowan Method
rinpol	1726.00		NIST Webbook
rinpol	1728.00		NIST Webbook
rinpol	1757.00		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=R320959&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

Latest version available from:
<https://www.chemeo.com/cid/75-204-2/Chromolaenin.pdf>

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