

Dihydrocrassifolone

Inchi: InChI=1S/C15H22O2/c1-11(2)9-13(16)10-15(3)7-4-5-12-6-8-17-14(12)15/h6,8,11H,4-5,7
InchiKey: RHZIPSSDEQVWHI-UHFFFAOYSA-N
Formula: C15H22O2
SMILES: CC(C)CC(=O)CC1(C)CCCc2ccoc21
Mol. weight [g/mol]: 234.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.35		Crippen Method
logp	3.879		Crippen Method
mcvol	199.330	ml/mol	McGowan Method
rinpol	1597.00		NIST Webbook
rinpol	1597.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R416649&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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
rinpol: Non-polar retention indices

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