

Crassifolone

Inchi: InChI=1S/C15H20O2/c1-11(2)9-13(16)10-15(3)7-4-5-12-6-8-17-14(12)15/h6,8-9H,4-5,7,11H
InchiKey: JYLMRMOUDBJDJU-UHFFFAOYSA-N
Formula: C15H20O2
SMILES: CC(C)=CC(=O)CC1(C)CCCc2ccoc21
Mol. weight [g/mol]: 232.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.44		Crippen Method
logp	3.799		Crippen Method
mcvol	195.030	ml/mol	McGowan Method
rinpol	1651.00		NIST Webbook
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Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R416634&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/13-395-9/Crassifolone.pdf>

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