

8-geranyloxypsoralen

Inchi: InChI=1S/C21H22O4/c1-14(2)5-4-6-15(3)9-11-24-21-16-7-8-20(22)25-19(16)13-18-17(2)
InchiKey: DBMJZOMNXBSRED-OQLLNIDSSA-N
Formula: C₂₁H₂₂O₄
SMILES: CC(C)=CCCC(C)=CCOc1c2ccoc2cc2oc(=O)ccc12
Mol. weight [g/mol]: 338.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-15.56		Crippen Method
logp	5.611		Crippen Method
mcvol	263.250	ml/mol	McGowan Method
rinpol	2865.00		NIST Webbook
rinpol	2865.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R422312&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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<https://www.chemeo.com/cid/84-665-1/8-geranyloxypsoralen.pdf>

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