

Naginatone

Inchi: InChI=1S/C10H14O2/c1-7(2)9(11)6-10-8(3)4-5-12-10/h4-5,7H,6H2,1-3H3
InchiKey: CIRYWPWWBAJBA-UHFFFAOYSA-N
Formula: C10H14O2
SMILES: Cc1ccoc1CC(=O)C(C)C
Mol. weight [g/mol]: 166.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.78		Crippen Method
logp	2.356		Crippen Method
mcvol	139.740	ml/mol	McGowan Method

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=R410765&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/75-896-5/Naginatone.pdf>

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