«beta»-Naginatene

Inchi: InChI=1S/C10H14O/c1-8(2)4-5-10-9(3)6-7-11-10/h6-7H,1,4-5H2,2-3H3
InchiKey: OGQMYOKLFYJRGZ-UHFFFAOYSA-N
Formula: C10H14O
SMILES: C=C(C)CCc1occc1C
Mol. weight [g/mol]: 150.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.59		Crippen Method
logp	3.097		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
rinpol	1095.00		NIST Webbook
rinpol	1095.00		NIST Webbook
ripol	1386.00		NIST Webbook
ripol	1386.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R409146&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
ripol: Polar retention indices