«beta»-Naginatene epoxide

Inchi: InChI=1S/C10H14O2/c1-8-4-6-11-9(8)3-5-10(2)7-12-10/h4,6H,3,5,7H2,1-2H3
InchiKey: ZDRYPNTZRDIHHL-UHFFFAOYSA-N
Formula: C10H14O2
SMILES: Cc1ccoc1CCC1(C)CO1
Mol. weight [g/mol]: 166.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.83		Crippen Method
logp	2.310		Crippen Method
mcvol	133.180	ml/mol	McGowan Method
rinpol	1170.00		NIST Webbook
ripol	1587.00		NIST Webbook
ripol	1587.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R409151&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

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