Davanafuran

Inchi: InChI=1S/C13H18O2/c1-4-13(3)8-7-12(15-13)10(2)11-6-5-9-14-11/h4-6,9-10,12H,1,7-8H
InchiKey: WBNXESGNGNWXSU-UHFFFAOYSA-N
Formula: C13H18O2
SMILES: C=CC1(C)CCC(C(C)c2ccco2)O1
Mol. weight [g/mol]: 206.28
CAS: 869379-85-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.96		Crippen Method
logp	3.507		Crippen Method
mcvol	171.150	ml/mol	McGowan Method
rinpol	1418.20		NIST Webbook
rinpol	1418.20		NIST Webbook

Sources

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=C869379851&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices