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-RDWQBYKPSA-N
Formula: C13H18O2
SMILES: C=CC1(C)CCC(C(C)c2ccco2)O1
Mol. weight [g/mol]: 206.28

Physical Properties

Property code	Value	Unit	Source
logp	3.507		Crippen Method
mcvol	171.150	ml/mol	McGowan Method
rinpol	1399.00		NIST Webbook
rinpol	1386.00		NIST Webbook
rinpol	1419.00		NIST Webbook
rinpol	1389.00		NIST Webbook
rinpol	1419.00		NIST Webbook
rinpol	1386.00		NIST Webbook
rinpol	1399.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R89548&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices