Furopelargone B

Inchi: InChI=1S/C15H22O2/c1-9(2)12-7-8-17-15(12)14-10(3)5-6-13(14)11(4)16/h7-10,13-14H,5

InchiKey: DVIZGXBTTFXQQC-UHFFFAOYSA-N

Formula: C15H22O2

SMILES: CC(=O)C1CCC(C)C1c1occc1C(C)C

Mol. weight [g/mol]: 234.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.36		Crippen Method
logp	4.122		Crippen Method
mcvol	199.330	ml/mol	McGowan Method
rinpol	1571.00		NIST Webbook
rinpol	1567.00		NIST Webbook
rinpol	1566.00		NIST Webbook
rinpol	1566.00		NIST Webbook
ripol	2065.00		NIST Webbook
ripol	2109.00		NIST Webbook
ripol	2109.00		NIST Webbook
ripol	2109.00		NIST Webbook
ripol	2121.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=R200607&Units=SI

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