

Furopelargone A

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-DDTOSNHZSA-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	1540.00		NIST Webbook
rinpol	1528.00		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=R199136&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

Latest version available from:

<https://www.chemeo.com/cid/58-542-6/Furopelargone-A.pdf>

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