furanoeremophil-1-one

Inchi: InChI=1S/C15H20O2/c1-9-8-17-14-6-12-13(16)5-4-10(2)15(12,3)7-11(9)14/h8,10,12H,4-
InchiKey: MHEQQQWHNMVBFL-GGYMPCQUSA-N
Formula: C15H20O2
SMILES: Cc1coc2c1CC1(C)C(C)CCC(=O)C1C2
Mol. weight [g/mol]: 232.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.14		Crippen Method
logp	3.308		Crippen Method
mcvol	188.470	ml/mol	McGowan Method
ripol	2706.00		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=R395443&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
ripol: Polar retention indices