5,5-Pentamethylene-2-phenyl-4-acetyl-1,3,4-oxadi

Inchi: InChI=1S/C15H18N2O2/c1-12(18)17-15(10-6-3-7-11-15)19-14(16-17)13-8-4-2-5-9-13/h2
InchiKey: LUIBSMWFXUWKLK-UHFFFAOYSA-N
Formula: C15H18N2O2
SMILES: CC(=O)N1N=C(c2ccccc2)OC12CCCCC2
Mol. weight [g/mol]: 258.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.78		Crippen Method
logp	2.887		Crippen Method
mcvol	199.830	ml/mol	McGowan Method
rinpol	2010.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R116691&Units=SI
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

Legend

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