5,5-Dimethyl-2-phenyl-4-acetyl-1,3,4-oxadiazoline

Inchi: InChI=1S/C12H14N2O2/c1-9(15)14-12(2,3)16-11(13-14)10-7-5-4-6-8-10/h4-8H,1-3H3
InchiKey: CSNFTOTUZCWEIG-UHFFFAOYSA-N
Formula: C12H14N2O2
SMILES: CC(=O)N1N=C(c2ccccc2)OC1(C)C
Mol. weight [g/mol]: 218.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.63		Crippen Method
logp	1.963		Crippen Method
mcvol	168.420	ml/mol	McGowan Method
rinpol	1560.00		NIST Webbook
rinpol	1560.00		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=R116671&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.