2,5-Dimethyl-4-benzoyl-1,3,4-oxadiazoline

Inchi: InChI=1S/C11H12N2O2/c1-8-12-13(9(2)15-8)11(14)10-6-4-3-5-7-10/h3-7,9H,1-2H3
InchiKey: AHMWEDKKIVQCLU-UHFFFAOYSA-N
Formula: C11H12N2O2
SMILES: CC1=NN(C(=O)c2ccccc2)C(C)O1
Mol. weight [g/mol]: 204.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.69		Crippen Method
logp	1.838		Crippen Method
mcvol	154.330	ml/mol	McGowan Method
rinpol	1540.00		NIST Webbook
rinpol	1540.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R116582&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

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