5,5-Dimethyl-2-phenyl-4-propionyl-1,3,4-oxadiazol

Inchi: InChI=1S/C13H16N2O2/c1-4-11(16)15-13(2,3)17-12(14-15)10-8-6-5-7-9-10/h5-9H,4H2,1
InchiKey: JJIXJTDOKAFPGX-UHFFFAOYSA-N
Formula: C13H16N2O2
SMILES: CCC(=O)N1N=C(c2ccccc2)OC1(C)C
Mol. weight [g/mol]: 232.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.05		Crippen Method
logp	2.353		Crippen Method
mcvol	182.510	ml/mol	McGowan Method
rinpol	1630.00		NIST Webbook
rinpol	1630.00		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=R116686&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

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