2-Pyrazoline, 4,4-dimethyl-5-(1-methylethyl), 1-benzoyl

Inchi: InChI=1S/C15H20N2O/c1-11(2)13-15(3,4)10-16-17(13)14(18)12-8-6-5-7-9-12/h5-11,13H

InchiKey: VSDNWFKINBKURY-UHFFFAOYSA-N

Formula: C15H20N2O

SMILES: CC(C)C1N(C(=O)c2ccccc2)N=CC1(C)C

Mol. weight [g/mol]: 244.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.80		Crippen Method
logp	3.179		Crippen Method
mcvol	204.820	ml/mol	McGowan Method
rinpol	1856.00		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=R322955&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