Pyrazol, 3(5)-butyl-5(3)-methyl, 1-benzoyl

Inchi: InChI=1S/C15H18N2O/c1-3-4-10-14-11-12(2)17(16-14)15(18)13-8-6-5-7-9-13/h5-9,11H,
InchiKey: XWYRSEQDTKROAV-UHFFFAOYSA-N
Formula: C15H18N2O
SMILES: CCCCc1cc(C)n(C(=O)c2ccccc2)n1
Mol. weight [g/mol]: 242.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.77		Crippen Method
logp	3.223		Crippen Method
mcvol	200.520	ml/mol	McGowan Method
rinpol	1873.00		NIST Webbook
rinpol	1873.00		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=R323205&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

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