Pyrazole, 3(5)-butyl-5(3)-methyl, 1-acetyl

Inchi: InChI=1S/C10H16N2O/c1-4-5-6-10-7-8(2)12(11-10)9(3)13/h7H,4-6H2,1-3H3
InchiKey: PRFXWDSGEOVVMX-UHFFFAOYSA-N
Formula: C10H16N2O
SMILES: CCCCc1cc(C)n(C(C)=O)n1
Mol. weight [g/mol]: 180.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.47		Crippen Method
logp	2.194		Crippen Method
mcvol	153.830	ml/mol	McGowan Method
rinpol	1311.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R323210&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices