

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
rinpola	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.cheméo.com/doc/models/crippen_log10ws

Legend

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

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