3(5)-methyl-5(3)-t-butylpyrazole

Inchi: InChI=1S/C8H14N2/c1-6-5-7(10-9-6)8(2,3)4/h5H,1-4H3,(H,9,10)
InchiKey: CUJNZTKYZLLKBY-UHFFFAOYSA-N
Formula: C8H14N2
SMILES: Cc1cc(C(C)(C)C)[nH]n1
Mol. weight [g/mol]: 138.21
CAS: 96440-80-1

Physical Properties

Property code	Value	Unit	Source
affp	946.20	kJ/mol	NIST Webbook
basg	914.30	kJ/mol	NIST Webbook
log10ws	-2.25		Crippen Method
logp	1.534		Crippen Method
mcvol	124.080	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C96440801&Units=SI

Legend

affp: Proton affinity
basg: Gas basicity
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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