1-methyl-5-t-butylpyrazole

Inchi: InChI=1S/C8H14N2/c1-8(2,3)7-5-6-9-10(7)4/h5-6H,1-4H3
InchiKey: ALCTZBPSAKAYDD-UHFFFAOYSA-N
Formula: C8H14N2
SMILES: Cn1nccc1C(C)(C)C
Mol. weight [g/mol]: 138.21
CAS: 141665-17-0

Physical Properties

Property code	Value	Unit	Source
affp	939.20	kJ/mol	NIST Webbook
basg	907.30	kJ/mol	NIST Webbook
log10ws	-3.84		Crippen Method
logp	1.718		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=C141665170&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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