

# 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/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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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