

# 1-methyl-3,5-di-t-butylpyrazole

**Inchi:** InChI=1S/C12H22N2/c1-11(2,3)9-8-10(12(4,5)6)14(7)13-9/h8H,1-7H3  
**InchiKey:** HOPUBWIABHRCKQ-UHFFFAOYSA-N  
**Formula:** C12H22N2  
**SMILES:** Cn1nc(C(C)(C)C)cc1C(C)(C)C  
**Mol. weight [g/mol]:** 194.32  
**CAS:** 141665-18-1

## Physical Properties

Property code	Value	Unit	Source
affp	970.80	kJ/mol	NIST Webbook
basg	937.10	kJ/mol	NIST Webbook
log10ws	-5.15		Crippen Method
logp	3.015		Crippen Method
mcvol	180.440	ml/mol	McGowan Method

## Sources

**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=C141665181&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## 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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