

1H-Pyrazole, 3,5-bis(1,1-dimethylethyl)-4-methyl-

Other names:	3,5-di-tert-Butyl-4-methyl-1H-pyrazole 3,5-di-t-Butyl-4-methylpyrazole
Inchi:	InChI=1S/C12H22N2/c1-8-9(11(2,3)4)13-14-10(8)12(5,6)7/h1-7H3,(H,13,14)
InchiKey:	HHGNOUNFOWXKFN-UHFFFAOYSA-N
Formula:	C12H22N2
SMILES:	Cc1c(C(C)(C)C)n[nH]c1C(C)(C)C
Mol. weight [g/mol]:	194.32
CAS:	18712-47-5

Physical Properties

Property code	Value	Unit	Source
affp	967.50	kJ/mol	NIST Webbook
basg	933.80	kJ/mol	NIST Webbook
log10ws	-3.56		Crippen Method
logp	2.831		Crippen Method
mcvol	180.440	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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18712475&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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