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/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=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