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

Other names: 3,5-di-t-Butylpyrazole
Inchi: InChI=1S/C11H20N2/c1-10(2,3)8-7-9(13-12-8)11(4,5)6/h7H,1-6H3,(H,12,13)
InchiKey: UEQDCVLVDQENIN-UHFFFAOYSA-N
Formula: C11H20N2
SMILES: CC(C)(C)c1cc(C(C)(C)C)[nH]n1
Mol. weight [g/mol]: 180.29
CAS: 1132-14-5

Physical Properties

Property code	Value	Unit	Source
affp	952.70	kJ/mol	NIST Webbook
basg	920.80	kJ/mol	NIST Webbook
log10ws	-3.08		Crippen Method
logp	2.523		Crippen Method
mcvol	166.350	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1132145&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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