1,4-dimethyl-3,5-di-t-butylpyrazole

Inchi: InChI=1S/C13H24N2/c1-9-10(12(2,3)4)14-15(8)11(9)13(5,6)7/h1-8H3
InchiKey: PNGZHMZNRTWVPT-UHFFFAOYSA-N
Formula: C13H24N2
SMILES: Cc1c(C(C)(C)C)nn(C)c1C(C)(C)C
Mol. weight [g/mol]: 208.34
CAS: 141665-20-5

Physical Properties

Property code	Value	Unit	Source
affp	979.60	kJ/mol	NIST Webbook
basg	947.80	kJ/mol	NIST Webbook
log10ws	-5.63		Crippen Method
logp	3.324		Crippen Method
mcvol	194.530	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=C141665205&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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