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
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/ci990307l

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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