1-methyl-3-t-butylpyrazole

Inchi: InChI=1S/C8H14N2/c1-8(2,3)7-5-6-10(4)9-7/h5-6H,1-4H3
InchiKey: LWFMELWSMBFNST-UHFFFAOYSA-N
Formula: C8H14N2
SMILES: Cn1ccc(C(C)(C)C)n1
Mol. weight [g/mol]: 138.21
CAS: 141665-16-9

Physical Properties

Property code	Value	Unit	Source
affp	944.40	kJ/mol	NIST Webbook
basg	912.50	kJ/mol	NIST Webbook
log10ws	-3.84		Crippen Method
logp	1.718		Crippen Method
mcvol	124.080	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=C141665169&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