3(5)-t-butylpyrazole

Inchi: InChI=1S/C7H12N2/c1-7(2,3)6-4-5-8-9-6/h4-5H,1-3H3,(H,8,9)
InchiKey: YIDCITOHTLPMMZ-UHFFFAOYSA-N
Formula: C7H12N2
SMILES: CC(C)(C)c1cc[nH]n1
Mol. weight [g/mol]: 124.18
CAS: 15802-80-9

Physical Properties

Property code	Value	Unit	Source
affp	922.80	kJ/mol	NIST Webbook
basg	891.00	kJ/mol	NIST Webbook
log10ws	-1.77		Crippen Method
logp	1.225		Crippen Method
mcvol	109.990	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=C15802809&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