1-t-Butylimidazole

Inchi: InChI=1S/C7H12N2/c1-7(2,3)9-5-4-8-6-9/h4-6H,1-3H3
InchiKey: AMQKPABOPFXDQM-UHFFFAOYSA-N
Formula: C7H12N2
SMILES: CC(C)(C)n1ccnc1
Mol. weight [g/mol]: 124.18
CAS: 45676-04-8

Physical Properties

Property code	Value	Unit	Source
affp	987.00	kJ/mol	NIST Webbook
basg	954.90	kJ/mol	NIST Webbook
log10ws	-2.01		Crippen Method
logp	1.638		Crippen Method
mcvol	109.990	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=C45676048&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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