

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/ci9903071>
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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