

1H-Imidazole, 1-butyl-4-methyl

Inchi: InChI=1S/C8H14N2/c1-3-4-5-10-6-8(2)9-7-10/h6-7H,3-5H2,1-2H3
InchiKey: AEMJJEJBDDKEPC-UHFFFAOYSA-N
Formula: C8H14N2
SMILES: CCCCN1cnc(C)c1
Mol. weight [g/mol]: 138.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.81		Crippen Method
logp	1.992		Crippen Method
mcvol	124.080	ml/mol	McGowan Method
rinpole	1218.00		NIST Webbook
ripole	1858.00		NIST Webbook
ripole	1858.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R68295&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpole: Non-polar retention indices
ripole: Polar retention indices

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