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
rinpol	1218.00		NIST Webbook
ripol	1858.00		NIST Webbook
ripol	1858.00		NIST Webbook

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=R68295&Units=SI

Legend

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

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