1H-Pyrrole, 2-butyl-1-methyl

Inchi: InChI=1S/C9H15N/c1-3-4-6-9-7-5-8-10(9)2/h5,7-8H,3-4,6H2,1-2H3
InchiKey: GXOVHTZKWWOSDN-UHFFFAOYSA-N
Formula: C9H15N
SMILES: CCCCc1cccn1C
Mol. weight [g/mol]: 137.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.40		Crippen Method
logp	2.368		Crippen Method
mcvol	128.190	ml/mol	McGowan Method
rinpol	1153.00		NIST Webbook
rinpol	1154.00		NIST Webbook
rinpol	1154.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R62720&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol: Non-polar retention indices