2-methyl-5-n-propylpyridine

Inchi: InChI=1S/C9H13N/c1-3-4-9-6-5-8(2)10-7-9/h5-7H,3-4H2,1-2H3
InchiKey: YLNFRYAOCLTTNL-UHFFFAOYSA-N
Formula: C9H13N
SMILES: CCCc1ccc(C)nc1
Mol. weight [g/mol]: 135.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.93		Crippen Method
logp	2.343		Crippen Method
mcvol	123.890	ml/mol	McGowan Method
ripol	1494.00		NIST Webbook
ripol	1491.00		NIST Webbook
ripol	1494.00		NIST Webbook
ripol	1494.00		NIST Webbook
ripol	1491.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R296836&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
ripol: Polar retention indices