Pyridine, 2-methyl-5-(1-methylethyl)

Inchi: InChI=1S/C9H13N/c1-7(2)9-5-4-8(3)10-6-9/h4-7H,1-3H3
InchiKey: WXASMDVSGYHPAH-UHFFFAOYSA-N
Formula: C9H13N
SMILES: Cc1ccc(C(C)C)cn1
Mol. weight [g/mol]: 135.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.90		Crippen Method
logp	2.513		Crippen Method
mcvol	123.890	ml/mol	McGowan Method
rinpol	1116.00		NIST Webbook
rinpol	1116.00		NIST Webbook
ripol	1610.00		NIST Webbook
ripol	1610.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R70482&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
ripol: Polar retention indices