Pyridine, 5-ethyl-2,4-dimethyl

Inchi: InChI=1S/C9H13N/c1-4-9-6-10-8(3)5-7(9)2/h5-6H,4H2,1-3H3
InchiKey: HDNSOESVSNPVNA-UHFFFAOYSA-N
Formula: C9H13N
SMILES: CCc1cnc(C)cc1C
Mol. weight [g/mol]: 135.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.99		Crippen Method
logp	2.261		Crippen Method
mcvol	123.890	ml/mol	McGowan Method
rinpol	1125.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1125.00		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=R53589&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