1,4,4-(CH3)3-1,2,3,4-tetrahydropyridine

Inchi: InChI=1S/C8H15N/c1-8(2)4-6-9(3)7-5-8/h4,6H,5,7H2,1-3H3
InchiKey: OBNANVWKTAVJEL-UHFFFAOYSA-N
Formula: C8H15N
SMILES: CN1C=CC(C)(C)CC1
Mol. weight [g/mol]: 125.21
CAS: 35079-50-6

Physical Properties

Property code	Value	Unit	Source
affp	979.90	kJ/mol	NIST Webbook
basg	947.30	kJ/mol	NIST Webbook
log10ws	-1.74		Crippen Method
logp	1.862		Crippen Method
mcvol	118.400	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C35079506&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp: Proton affinity
basg: Gas basicity
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume