2-(chloromethyl)-1-methylpiperidine

Other names: c-C5H9N,2-CH2Cl,1-CH3
Inchi: InChI=1S/C7H14ClN/c1-9-5-3-2-4-7(9)6-8/h7H,2-6H2,1H3
InchiKey: FGMRHGUEOYXVMX-UHFFFAOYSA-N
Formula: C7H14ClN
SMILES: CN1CCCCC1CCl
Mol. weight [g/mol]: 147.65
CAS: 49665-74-9

Physical Properties

Property code	Value	Unit	Source
affp	965.00	kJ/mol	NIST Webbook
basg	934.20	kJ/mol	NIST Webbook
log10ws	-1.48		Crippen Method
logp	1.710		Crippen Method
mcvol	120.850	ml/mol	McGowan Method

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=C49665749&Units=SI

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