1-Methyl-1,2,3,6-tetrahydropyridine

Other names:	Pyridine, 1,2,3,6-tetrahydro-1-methyl-
	N-Methyl-1,2,5,6-tetrahydropyridine
	1-Methyl-3-piperideine
	1,2,3,4-tetrahydro-1-methylpyridine
Inchi:	InChI=1S/C6H11N/c1-7-5-3-2-4-6-7/h2-3H,4-6H2,1H3
InchiKey:	AUFIRGPROMANKW-UHFFFAOYSA-N
Formula:	C6H11N
SMILES:	CN1CC=CCC1
Mol. weight [g/mol]:	97.16
CAS:	694-55-3

Physical Properties

Property code	Value	Unit	Source
ie	8.67 ± 0.05	eV	NIST Webbook
log10ws	-0.65		Crippen Method
logp	0.878		Crippen Method
mcvol	90.220	ml/mol	McGowan Method
ripol	1030.00		NIST Webbook
ripol	1030.00		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=C694553&Units=SI

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

ripol: Polar retention indices