1-Methyl-hexahydroazepine

Other names:	hexahydro-1-methyl-1H-azepine
	1H-Azepine, hexahydro-1-methyl-
Inchi:	InChI=1S/C7H15N/c1-8-6-4-2-3-5-7-8/h2-7H2,1H3
InchiKey:	ZKUKXSWKWGHYKJ-UHFFFAOYSA-N
Formula:	C7H15N
SMILES:	CN1CCCCCC1
Mol. weight [g/mol]:	113.20
CAS:	1192-95-6

Physical Properties

Property code	Value	Unit	Source
ie	8.29 ± 0.02	eV	NIST Webbook
log10ws	-1.22		Crippen Method
logp	1.492		Crippen Method
mcvol	108.610	ml/mol	McGowan Method
rinpol	882.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1192956&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices