1-Azabicyclo[2.2.2]octane, 3-methyl-

Other names:	Quinuclidine, 3-methyl- 3-Methylquinuclidine
Inchi:	InChI=1S/C8H15N/c1-7-6-9-4-2-8(7)3-5-9/h7-8H,2-6H2,1H3
InchiKey:	MWBULQNPGVGHKO-UHFFFAOYSA-N
Formula:	C8H15N
SMILES:	CC1CN2CCC1CC2
Mol. weight [g/mol]:	125.21
CAS:	695-88-5

Physical Properties

Property code	Value	Unit	Source
affp	982.50	kJ/mol	NIST Webbook
basg	951.70	kJ/mol	NIST Webbook
log10ws	-1.05		Crippen Method
logp	1.348		Crippen Method
mcvol	111.840	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=C695885&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

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