

1-Azabicyclo[2.2.2]octane, 2-methyl-

Other names:	Quinuclidine, 2-methyl- 2-Methylquinuclidine
Inchi:	InChI=1S/C8H15N/c1-7-6-8-2-4-9(7)5-3-8/h7-8H,2-6H2,1H3
InchiKey:	VDWODSPSMJMZQI-UHFFFAOYSA-N
Formula:	C8H15N
SMILES:	CC1CC2CCN1CC2
Mol. weight [g/mol]:	125.21
CAS:	5261-65-4

Physical Properties

Property code	Value	Unit	Source
affp	986.90	kJ/mol	NIST Webbook
basg	956.10	kJ/mol	NIST Webbook
log10ws	-1.40		Crippen Method
logp	1.491		Crippen Method
mcvol	111.840	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=C5261654&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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