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/ci990307l
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