3-Chloro-1-azabicyclo[2.2.2]octane

Inchi: InChI=1S/C7H12ClN/c8-7-5-9-3-1-6(7)2-4-9/h6-7H,1-5H2
InchiKey: NOLVABYTFMDREN-UHFFFAOYSA-N
Formula: C7H12ClN
SMILES: ClC1CN2CCC1CC2
Mol. weight [g/mol]: 145.63
CAS: 42332-45-6

Physical Properties

Property code	Value	Unit	Source
affp	954.30	kJ/mol	NIST Webbook
basg	923.50	kJ/mol	NIST Webbook
ie	8.80	eV	NIST Webbook
log10ws	-1.14		Crippen Method
logp	1.319		Crippen Method
mcvol	109.990	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=C42332456&Units=SI

Legend

affp: Proton affinity
basg: Gas basicity
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume