3-Amino-1-azabicyclo[2.2.2]octane

Other names: (+-)-3-Aminoquinuclidine
Inchi: InChI=1S/C7H14N2/c8-7-5-9-3-1-6(7)2-4-9/h6-7H,1-5,8H2
InchiKey: REUAXQZIRFXQML-UHFFFAOYSA-N
Formula: C7H14N2
SMILES: NC1CN2CCC1CC2
Mol. weight [g/mol]: 126.20
CAS: 6238-14-8

Physical Properties

Property code	Value	Unit	Source
affp	985.50	kJ/mol	NIST Webbook
basg	954.70	kJ/mol	NIST Webbook
ie	7.96	eV	NIST Webbook
log10ws	-0.42		Crippen Method
logp	0.039		Crippen Method
mcvol	107.730	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6238148&Units=SI
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

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