4-Chloro-1-azabicyclo[2.2.2]octane

Other names: 1-Azabicyclo[2.2.2]octane,4-chloro-
Inchi: InChI=1S/C7H12ClN/c8-7-1-4-9(5-2-7)6-3-7/h1-6H2
InchiKey: CHAXYLNTCZVHBJ-UHFFFAOYSA-N
Formula: C7H12ClN
SMILES: ClC12CCN(CC1)CC2
Mol. weight [g/mol]: 145.63
CAS: 5960-95-2

Physical Properties

Property code	Value	Unit	Source
affp	949.40	kJ/mol	NIST Webbook
basg	918.60	kJ/mol	NIST Webbook
ie	8.55 ± 0.01	eV	NIST Webbook
log10ws	-1.38		Crippen Method
logp	1.463		Crippen Method
mcvol	109.990	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5960952&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