1-azabicyclo[2.2.2]-octane, 2-chloro

Inchi: InChI=1S/C7H12ClN/c8-7-5-6-1-3-9(7)4-2-6/h6-7H,1-5H2
InchiKey: BZYQYFBFBXSMHK-UHFFFAOYSA-N
Formula: C7H12ClN
SMILES: ClC1CC2CCN1CC2
Mol. weight [g/mol]: 145.63
CAS: 96943-88-3

Physical Properties

Property code	Value	Unit	Source
affp	950.80	kJ/mol	NIST Webbook
basg	920.00	kJ/mol	NIST Webbook
log10ws	-1.63		Crippen Method
logp	1.667		Crippen Method
mcvol	109.990	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C96943883&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
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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