

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:	<chem>C1C12CCN(CC1)CC2</chem>
Mol. weight [g/mol]:	145.63

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
logp	1.464		Crippen Method
mcvol	109.990	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5960952&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

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