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

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
logp	1.319		Crippen Method
mcvol	109.990	ml/mol	McGowan Method
tb	469.78	K	Cheméo Relay (1.0)
tf	444.86	K	Cheméo Relay (1.0)

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=C42332456&Units=SI

Legend

affp: Proton affinity
basg: Gas basicity
ie: Ionization energy
logp: Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point