1-Azabicyclo[2.2.2]octane, 4-methyl-

Other names: 4-Methyl-1-azabicyclo[2.2.2]octane
Inchi: InChI=1S/C8H15N/c1-8-2-5-9(6-3-8)7-4-8/h2-7H2,1H3
InchiKey: DLHGEIMBTIHQGR-UHFFFAOYSA-N
Formula: C8H15N
SMILES: CC12CCN(CC1)CC2
Mol. weight [g/mol]: 125.21
CAS: 45651-41-0

Physical Properties

Property code	Value	Unit	Source
affp	979.40	kJ/mol	NIST Webbook
basg	948.60	kJ/mol	NIST Webbook
ie	8.06 ± 0.01	eV	NIST Webbook
log10ws	-1.29		Crippen Method
logp	1.492		Crippen Method
mcvol	111.840	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C45651410&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