1-Azabicyclo[2.2.2]octane-4-methanol

Other names: 4-(Hydroxymethyl)-1-azabicyclo[2.2.2]octane
Inchi: InChI=1S/C8H15NO/c10-7-8-1-4-9(5-2-8)6-3-8/h10H,1-7H2
InchiKey: PGGCTNQYCZTVNL-UHFFFAOYSA-N
Formula: C8H15NO
SMILES: OCC12CCN(CC1)CC2
Mol. weight [g/mol]: 141.21
CAS: 26608-58-2

Physical Properties

Property code	Value	Unit	Source
ie	8.17 ± 0.01	eV	NIST Webbook
log10ws	-0.55		Crippen Method
logp	0.465		Crippen Method
mcvol	117.710	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C26608582&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume