1-Azabicyclo[2.2.2]octan-4-ol

Inchi: InChI=1S/C7H13NO/c9-7-1-4-8(5-2-7)6-3-7/h9H,1-6H2
InchiKey: RQRSQXFVRUWISR-UHFFFAOYSA-N
Formula: C7H13NO
SMILES: OC12CCN(CC1)CC2
Mol. weight [g/mol]: 127.18
CAS: 26458-74-2

Physical Properties

Property code	Value	Unit	Source
ie	8.48 ± 0.01	eV	NIST Webbook
log10ws	-0.49		Crippen Method
logp	0.217		Crippen Method
mcvol	103.620	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C26458742&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

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.