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

Inchi: InChI=1S/C13H17N/c1-2-4-12(5-3-1)13-6-9-14(10-7-13)11-8-13/h1-5H,6-11H2
InchiKey: CSKNWIPXDBBWRW-UHFFFAOYSA-N
Formula: C13H17N
SMILES: c1ccc(C23CCN(CC2)CC3)cc1
Mol. weight [g/mol]: 187.28
CAS: 51069-11-5

Physical Properties

Property code	Value	Unit	Source
ie	8.13 ± 0.01	eV	NIST Webbook
log10ws	-2.40		Crippen Method
logp	2.424		Crippen Method
mcvol	158.530	ml/mol	McGowan Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C51069115&Units=SI

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.