Aziridine, 1-phenyl-

Other names: N-Phenylaziridine
N-Phenylethylenimine
1-Phenylaziridine
Inchi: InChI=1S/C8H9N/c1-2-4-8(5-3-1)9-6-7-9/h1-5H,6-7H2
InchiKey: YKNKBBMRKMLLJS-UHFFFAOYSA-N
Formula: C8H9N
SMILES: c1ccc(N2CC2)cc1
Mol. weight [g/mol]: 119.16
CAS: 696-18-4

Physical Properties

Property code	Value	Unit	Source
affp	926.50	kJ/mol	NIST Webbook
basg	895.70	kJ/mol	NIST Webbook
ie	8.00 ± 0.10	eV	NIST Webbook
ie	8.19 ± 0.06	eV	NIST Webbook
ie	8.10	eV	NIST Webbook
ie	8.00	eV	NIST Webbook
log10ws	-1.27		Crippen Method
logp	1.507		Crippen Method
mcvol	98.940	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=C696184&Units=SI

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