N-Phenylpyrrolidine

Other names:	1-Phenylpyrrolidine
	Pyrrolidine, 1-phenyl-
Inchi:	InChI=1S/C10H13N/c1-2-6-10(7-3-1)11-8-4-5-9-11/h1-3,6-7H,4-5,8-9H2
InchiKey:	VDQQJMHXZCMNMU-UHFFFAOYSA-N
Formula:	C10H13N
SMILES:	c1ccc(N2CCCC2)cc1
Mol. weight [g/mol]:	147.22
CAS:	4096-21-3

Physical Properties

Property code	Value	Unit	Source
affp	941.60	kJ/mol	NIST Webbook
basg	915.10	kJ/mol	NIST Webbook
ie	6.80	eV	NIST Webbook
ie	7.23 ± 0.06	eV	NIST Webbook
log10ws	-2.11		Crippen Method
logp	2.287		Crippen Method
mcvol	127.120	ml/mol	McGowan Method

Sources

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=C4096213&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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