

N-Phenylpiperidine

Other names:	Piperidine, 1-phenyl- 1-Phenylpiperidine
Inchi:	InChI=1S/C11H15N/c1-3-7-11(8-4-1)12-9-5-2-6-10-12/h1,3-4,7-8H,2,5-6,9-10H2
InchiKey:	LLSKXGRDUPMXLC-UHFFFAOYSA-N
Formula:	C11H15N
SMILES:	<chem>c1ccc(N2CCCCC2)cc1</chem>
Mol. weight [g/mol]:	161.24
CAS:	4096-20-2

Physical Properties

Property code	Value	Unit	Source
affp	952.90	kJ/mol	NIST Webbook
basg	926.40	kJ/mol	NIST Webbook
hvap	64.30 ± 0.40	kJ/mol	NIST Webbook
ie	7.10	eV	NIST Webbook
ie	7.72 ± 0.06	eV	NIST Webbook
log10ws	-2.53		Crippen Method
logp	2.677		Crippen Method
mcvol	141.210	ml/mol	McGowan Method
tb	531.20	K	NIST Webbook
tb	530.65 ± 4.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	64.00 ± 0.40	kJ/mol	303.50	NIST Webbook

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=C4096202&Units=SI>

Legend

affp:	Proton affinity
basg:	Gas basicity
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature

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