1-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: c1ccc(N2CCCCC2)cc1
Mol. weight [g/mol]: 161.25

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
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
tf	273.90	K	Cheméo Relay (1.0)

Temperature Dependent Properties

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

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4096202&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point