Phenylcyclopentylamine

Other names: N-Cyclopentylaniline
Inchi: InChI=1S/C11H15N/c1-2-6-10(7-3-1)12-11-8-4-5-9-11/h1-3,6-7,11-12H,4-5,8-9H2
InchiKey: WEULTTCXSOUGPM-UHFFFAOYSA-N
Formula: C11H15N
SMILES: c1ccc(NC2CCCC2)cc1
Mol. weight [g/mol]: 161.24
CAS: 40649-26-1

Physical Properties

Property code	Value	Unit	Source
gf	280.09	kJ/mol	Joback Method
hf	80.11	kJ/mol	Joback Method
hfus	17.32	kJ/mol	Joback Method
hvap	49.05	kJ/mol	Joback Method
ie	7.45	eV	NIST Webbook
log10ws	-3.16		Crippen Method
logp	3.041		Crippen Method
mcvol	141.210	ml/mol	McGowan Method
pc	3265.31	kPa	Joback Method
tb	543.21	K	Joback Method
tc	778.87	K	Joback Method
tf	303.71	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.68	J/mol×K	543.21	Joback Method
cpg	356.66	J/mol×K	582.49	Joback Method
cpg	374.29	J/mol×K	621.76	Joback Method
cpg	390.62	J/mol×K	661.04	Joback Method
cpg	405.74	J/mol×K	700.31	Joback Method
cpg	419.71	J/mol×K	739.59	Joback Method
cpg	432.60	J/mol×K	778.87	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40649261&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume