N-Phenylcyclohexylamine

Other names:	N-Cyclohexylaniline Benzenamine, N-cyclohexyl- Aniline, N-cyclohexyl- Cyclohexanamine, N-phenyl- Cyclohexylamine, N-phenyl- Diphenylamine, ar-hexahydro- Cyclohexylphenylamine N-Cyclohexylbenzenamine Phenylcyclohexylamine NSC 27510
Inchi:	InChI=1S/C12H17N/c1-3-7-11(8-4-1)13-12-9-5-2-6-10-12/h1,3-4,7-8,12-13H,2,5-6,9-10H
InchiKey:	TXTHKGMZDDTZFD-UHFFFAOYSA-N
Formula:	C12H17N
SMILES:	c1ccc(NC2CCCCC2)cc1
Mol. weight [g/mol]:	175.27
CAS:	1821-36-9

Physical Properties

Property code	Value	Unit	Source
gf	276.41	kJ/mol	Joback Method
hf	53.31	kJ/mol	Joback Method
hfus	17.81	kJ/mol	Joback Method
hvap	51.45	kJ/mol	Joback Method
ie	7.45	eV	NIST Webbook
log10ws	-3.58		Crippen Method
logp	3.431		Crippen Method
mcvol	155.300	ml/mol	McGowan Method
pc	3015.64	kPa	Joback Method
tb	570.36	K	Joback Method
tc	809.89	K	Joback Method
tf	311.46	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.69	J/mol×K	570.36	Joback Method
cpg	408.29	J/mol×K	610.28	Joback Method
cpg	427.41	J/mol×K	650.20	Joback Method
cpg	445.11	J/mol×K	690.12	Joback Method
cpg	461.46	J/mol×K	730.04	Joback Method
cpg	476.54	J/mol×K	769.97	Joback Method
cpg	490.40	J/mol×K	809.89	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	464.70	K	9.70	NIST Webbook

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=C1821369&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume