N-(4-Chlorophenyl)-1,2-phenylenediamine

Other names:	1,2-Benzenediamine, N-(4-chlorophenyl)-
	N-(4-chlorophenyl)benzene-1,2-diamine
Inchi:	InChI=1S/C12H11ClN2/c13-9-5-7-10(8-6-9)15-12-4-2-1-3-11(12)14/h1-8,15H,14H2
InchiKey:	WEUBIWJPIRTWDF-UHFFFAOYSA-N
Formula:	C12H11ClN2
SMILES:	Nc1ccccc1Nc1ccc(Cl)cc1
Mol. weight [g/mol]:	218.68
CAS:	68817-71-0

Physical Properties

Property code	Value	Unit	Source
gf	399.63	kJ/mol	Joback Method
hf	230.63	kJ/mol	Joback Method
hfus	28.63	kJ/mol	Joback Method
hvap	69.64	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	3.666		Crippen Method
mcvol	164.620	ml/mol	McGowan Method
pc	3439.94	kPa	Joback Method
tb	697.41	K	Joback Method
tc	955.95	K	Joback Method
tf	468.72	K	Joback Method
vc	0.605	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.30	J/mol×K	697.41	Joback Method
cpg	419.32	J/mol×K	740.50	Joback Method
cpg	431.21	J/mol×K	783.59	Joback Method
cpg	442.03	J/mol×K	826.68	Joback Method
cpg	451.87	J/mol×K	869.77	Joback Method
cpg	460.80	J/mol×K	912.86	Joback Method
cpg	468.91	J/mol×K	955.95	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C68817710&Units=SI

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
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