p-Chloroaniline

Other names:	1-Amino-4-chlorobenzene
	4-Amino-1-chlorobenzene
	4-Aminochlorobenzene
	4-CHLORO-BENZENAMINE
	4-Chloranilin
	4-Chloro-1-aminobenzene
	4-Chloroaniline
	4-Chlorobenzenamine
	4-Chlorophenylamine
	Aniline, 4-chloro-
	Aniline, p-chloro-
	Benzenamine, 4-chloro-
	Benzeneamine, 4-chloro
	NCI-C02039
	NSC 36941
	P-AMINOCHLOROBENZENE
	Rcra waste number P024
	benzene, 1-amino-4-chloro-
	p-Ca
	p-Chloraniline
	p-Chlorophenylamine
Inchi:	InChI=1S/C6H6ClN/c7-5-1-3-6(8)4-2-5/h1-4H,8H2
InchiKey:	QSNSCYSYFYORTR-UHFFFAOYSA-N
Formula:	C6H6ClN
SMILES:	Nc1ccc(Cl)cc1
Mol. weight [g/mol]:	127.57
CAS:	106-47-8

Physical Properties

Property code	Value	Unit	Source
affp	873.80	kJ/mol	NIST Webbook
basg	842.00	kJ/mol	NIST Webbook
chl	-3339.00 ± 13.00	kJ/mol	NIST Webbook
chs	-3208.80 ± 1.90	kJ/mol	NIST Webbook
gf	156.94	kJ/mol	Joback Method
hf	75.94	kJ/mol	Joback Method

hfs	-33.30	kJ/mol	NIST Webbook
hfus	20.47	kJ/mol	Heat Capacities of Chloroanilines and Chloronitrobenzenes
hsub	80.50 ± 0.30	kJ/mol	NIST Webbook
hvap	62.30 ± 0.50	kJ/mol	NIST Webbook
hvap	48.95	kJ/mol	NIST Webbook
ie	8.18	eV	NIST Webbook
ie	7.80 ± 0.10	eV	NIST Webbook
ie	8.00	eV	NIST Webbook
log10ws	-1.66		Estimated Solubility Method
log10ws	-1.66		Aqueous Solubility Prediction Method
logp	1.922		Crippen Method
mcvol	93.860	ml/mol	McGowan Method
pc	4704.19	kPa	Joback Method
rinpol	202.80		NIST Webbook
rinpol	1198.00		NIST Webbook
rinpol	1157.00		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	202.80		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1201.00		NIST Webbook
rinpol	1204.00		NIST Webbook
rinpol	1204.00		NIST Webbook
rinpol	1161.00		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1159.00		NIST Webbook
ripol	2130.00		NIST Webbook
ripol	2100.00		NIST Webbook
ripol	2100.00		NIST Webbook
ripol	2100.00		NIST Webbook
tb	505.45 ± 1.00	K	NIST Webbook
tb	505.20	K	NIST Webbook
tc	716.47	K	Joback Method
tf	344.40	K	Aqueous Solubility Prediction Method
vc	0.342	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	171.54	J/mol×K	478.30	Joback Method
cpg	180.87	J/mol×K	517.99	Joback Method
cpg	189.55	J/mol×K	557.69	Joback Method
cpg	197.61	J/mol×K	597.38	Joback Method
cpg	205.09	J/mol×K	637.08	Joback Method
cpg	212.01	J/mol×K	676.77	Joback Method
cpg	218.41	J/mol×K	716.47	Joback Method
cps	147.30	J/mol×K	305.00	NIST Webbook
hfust	20.47	kJ/mol	342.80	NIST Webbook
hfust	16.90	kJ/mol	344.00	NIST Webbook
hsubt	90.70	kJ/mol	293.00	NIST Webbook
hvapt	52.20	kJ/mol	434.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49028e+01
Coeff. B	-4.46985e+03
Coeff. C	-7.05800e+01
Temperature range (K), min.	343.05
Temperature range (K), max.	536.61

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.42262e+01
Coeff. B	-1.00637e+04
Coeff. C	-9.73256e+00
Coeff. D	3.57991e-06
Temperature range (K), min.	343.05
Temperature range (K), max.	754.00

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1288.mol
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Thermochemistry of adducts of some bivalent transition metal bromides with 4-chloroaniline:	https://www.doi.org/10.1016/j.tca.2006.05.022
Heat Capacities of Chloroanilines and Chloronitrobenzenes:	https://www.doi.org/10.1021/je700080k
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106478&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1288

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume