m-Chloroaniline

Other names:	1-Amino-3-chlorobenzene
	3-CHLORO-BENZENAMINE
	3-Chlooranilinen
	3-Chloroaniline
	3-Chlorobenzenamine
	3-Chlorophenylamine
	3-Cloroaniline
	3-amino-1-chlorobenzene
	3-chloro-1-aminobenzene
	Aniline, 3-chloro-
	Aniline, m-chloro-
	Azoic diazo component 2, base
	Benzenamine, 3-chloro-
	Benzeneamine, 3-chloro-
	Fast Orange GC Base
	M-AMINOCHLOROBENZENE
	NSC 17581
	Orange GC base
	m-Chloraniline
	m-Chloroaminobenzene
	m-Chlorophenylamine
Inchi:	InChI=1S/C6H6ClN/c7-5-2-1-3-6(8)4-5/h1-4H,8H2
InchiKey:	PNPCRKVUWYDDST-UHFFFAOYSA-N
Formula:	C6H6ClN
SMILES:	Nc1cccc(Cl)c1
Mol. weight [g/mol]:	127.57
CAS:	108-42-9

Physical Properties

Property code	Value	Unit	Source
affp	868.10	kJ/mol	NIST Webbook
basg	836.30	kJ/mol	NIST Webbook
chl	-3221.80 ± 1.70	kJ/mol	NIST Webbook
chl	-3362.60 ± 2.70	kJ/mol	NIST Webbook
gf	156.94	kJ/mol	Joback Method
hf	75.94	kJ/mol	Joback Method

hfl	-20.30	kJ/mol	NIST Webbook
hfus	14.34	kJ/mol	Joback Method
hvap	54.00 ± 0.20	kJ/mol	NIST Webbook
hvap	61.10 ± 2.80	kJ/mol	NIST Webbook
hvap	60.20 ± 0.10	kJ/mol	NIST Webbook
ie	8.10 ± 0.10	eV	NIST Webbook
log10ws	-1.37		Estimated Solubility Method
log10ws	-1.37		Aqueous Solubility Prediction Method
logp	1.922		Crippen Method
mcvol	93.860	ml/mol	McGowan Method
pc	4704.19	kPa	Joback Method
rinpol	1157.00		NIST Webbook
rinpol	1201.00		NIST Webbook
rinpol	1198.00		NIST Webbook
rinpol	1157.00		NIST Webbook
rinpol	1160.60		NIST Webbook
rinpol	1160.60		NIST Webbook
rinpol	1155.00		NIST Webbook
rinpol	1156.00		NIST Webbook
rinpol	1204.00		NIST Webbook
rinpol	1201.00		NIST Webbook
rinpol	1157.00		NIST Webbook
rinpol	1157.00		NIST Webbook
rinpol	1204.00		NIST Webbook
rinpol	1158.00		NIST Webbook
rinpol	1204.00		NIST Webbook
rinpol	1156.00		NIST Webbook
ripol	2140.00		NIST Webbook
ripol	2110.00		NIST Webbook
ripol	2110.00		NIST Webbook
ripol	2110.00		NIST Webbook
tb	503.15 ± 1.50	K	NIST Webbook
tb	503.70 ± 2.00	K	NIST Webbook
tb	503.20	K	NIST Webbook
tb	509.65 ± 1.00	K	NIST Webbook
tc	716.47	K	Joback Method
tf	263.02	K	Aqueous Solubility Prediction Method
tf	263.15 ± 0.50	K	NIST Webbook
tf	262.90 ± 0.02	K	NIST Webbook
tf	262.80 ± 0.50	K	NIST Webbook
vc	0.342	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	197.61	J/mol×K	597.38	Joback Method
cpg	218.41	J/mol×K	716.47	Joback Method
cpg	212.01	J/mol×K	676.77	Joback Method
cpg	205.09	J/mol×K	637.08	Joback Method
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
cpl	210.90	J/mol×K	339.77	Heat Capacities of Chloroanilines and Chloronitrobenzenes
cpl	213.00	J/mol×K	349.98	Heat Capacities of Chloroanilines and Chloronitrobenzenes
cpl	212.90	J/mol×K	349.98	Heat Capacities of Chloroanilines and Chloronitrobenzenes
cpl	213.40	J/mol×K	349.98	Heat Capacities of Chloroanilines and Chloronitrobenzenes
cpl	200.30	J/mol×K	278.51	Heat Capacities of Chloroanilines and Chloronitrobenzenes
cpl	199.90	J/mol×K	278.51	Heat Capacities of Chloroanilines and Chloronitrobenzenes
cpl	201.80	J/mol×K	288.72	Heat Capacities of Chloroanilines and Chloronitrobenzenes
cpl	201.50	J/mol×K	288.72	Heat Capacities of Chloroanilines and Chloronitrobenzenes
cpl	204.00	J/mol×K	298.93	Heat Capacities of Chloroanilines and Chloronitrobenzenes
cpl	203.90	J/mol×K	298.93	Heat Capacities of Chloroanilines and Chloronitrobenzenes

cpl	203.50	J/mol×K	298.93	Heat Capacities of Chloroanilines and Chloronitrobenzenes
cpl	205.50	J/mol×K	309.14	Heat Capacities of Chloroanilines and Chloronitrobenzenes
cpl	205.30	J/mol×K	309.14	Heat Capacities of Chloroanilines and Chloronitrobenzenes
cpl	205.20	J/mol×K	309.14	Heat Capacities of Chloroanilines and Chloronitrobenzenes
cpl	207.60	J/mol×K	319.35	Heat Capacities of Chloroanilines and Chloronitrobenzenes
cpl	207.40	J/mol×K	319.35	Heat Capacities of Chloroanilines and Chloronitrobenzenes
cpl	198.70	J/mol×K	294.70	NIST Webbook
cpl	209.60	J/mol×K	329.56	Heat Capacities of Chloroanilines and Chloronitrobenzenes
cpl	209.40	J/mol×K	329.56	Heat Capacities of Chloroanilines and Chloronitrobenzenes
cpl	209.40	J/mol×K	329.56	Heat Capacities of Chloroanilines and Chloronitrobenzenes
cpl	211.10	J/mol×K	339.77	Heat Capacities of Chloroanilines and Chloronitrobenzenes
cpl	210.80	J/mol×K	339.77	Heat Capacities of Chloroanilines and Chloronitrobenzenes
cpl	207.40	J/mol×K	319.35	Heat Capacities of Chloroanilines and Chloronitrobenzenes
hfust	12.00	kJ/mol	263.00	NIST Webbook
hvapt	60.30 ± 0.60	kJ/mol	319.00	NIST Webbook
hvapt	61.00 ± 0.80	kJ/mol	323.00	NIST Webbook
hvapt	53.60	kJ/mol	485.50	NIST Webbook

rhol	1191.98	kg/m3	318.15	Study on thermo physical properties of binary mixture containing aromatic alcohol with aromatic, substituted aromatic amines at different temperatures interms of FT-IR, 1H NMR spectroscopic and DFT method
rhol	1205.32	kg/m3	303.15	Volumetric, acoustic and spectroscopic properties of 3-chloroaniline with substituted ethanols at various temperatures
rhol	1191.25	kg/m3	318.15	Volumetric, acoustic and spectroscopic properties of 3-chloroaniline with substituted ethanols at various temperatures
rhol	1200.75	kg/m3	308.15	Volumetric, acoustic and spectroscopic properties of 3-chloroaniline with substituted ethanols at various temperatures
rhol	1205.75	kg/m3	303.15	Study on thermo physical properties of binary mixture containing aromatic alcohol with aromatic, substituted aromatic amines at different temperatures interms of FT-IR, 1H NMR spectroscopic and DFT method

rhol	1201.14	kg/m3	308.15	Study on thermo physical properties of binary mixture containing aromatic alcohol with aromatic, substituted aromatic amines at different temperatures interms of FT-IR, 1H NMR spectroscopic and DFT method	
rhol	1196.56	kg/m3	313.15	Study on thermo physical properties of binary mixture containing aromatic alcohol with aromatic, substituted aromatic amines at different temperatures interms of FT-IR, 1H NMR spectroscopic and DFT method	
rhol	1196.02	kg/m3	313.15	Volumetric, acoustic and spectroscopic properties of 3-chloroaniline with substituted ethanols at various temperatures	
rhol	1187.41	kg/m3	323.15	Study on thermo physical properties of binary mixture containing aromatic alcohol with aromatic, substituted aromatic amines at different temperatures interms of FT-IR, 1H NMR spectroscopic and DFT method	
speedsl	1484.00	m/s	313.15	Thermodynamic and acoustic properties of binary mixtures of ethers. V. Diisopropyl ether or oxolane with 2- or 3-chloroanilines at 303.15, 313.15 and 323.15 K	

speedsl	1486.00	m/s	313.15	Thermodynamic and acoustic properties of binary mixtures of ethers. V. Diisopropyl ether or oxolane with 2- or 3-chloroanilines at 303.15, 313.15 and 323.15 K
speedsl	1452.00	m/s	323.15	Thermodynamic and acoustic properties of binary mixtures of ethers. V. Diisopropyl ether or oxolane with 2- or 3-chloroanilines at 303.15, 313.15 and 323.15 K
speedsl	1517.00	m/s	303.15	Thermodynamic and acoustic properties of binary mixtures of ethers. V. Diisopropyl ether or oxolane with 2- or 3-chloroanilines at 303.15, 313.15 and 323.15 K

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	368.70	K	1.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49069e+01
Coeff. B	-4.45692e+03
Coeff. C	-7.00090e+01
Temperature range (K), min.	374.87

Information	Value
Temperature range (K), max.	534.49

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.38199e+01
Coeff. B	-1.01999e+04
Coeff. C	-9.60275e+00
Coeff. D	3.14403e-06
Temperature range (K), min.	262.75
Temperature range (K), max.	751.00

Sources

Volumetric, acoustic and spectroscopic properties of 3-chloroaniline with substituted ethanols at various temperatures:	https://www.doi.org/10.1016/j.jct.2015.11.012
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C108429&Units=SI
Heat Capacities of Chloroanilines and Chloronitrobenzenes:	https://www.doi.org/10.1021/je700080k
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Study on thermo physical properties of binary mixture containing aromatic alcohol with aromatic, substituted aromatic amines at different temperatures in terms of FT-IR, 1H NMR spectroscopic and DFT method:	https://www.doi.org/10.1016/j.fluid.2018.01.025
Studies on the importance of nature of substituent on the thermodynamic and transport properties of liquid mixtures at various temperatures:	https://www.doi.org/10.1016/j.jct.2016.05.015
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1287
Thermodynamic and acoustic properties of binary mixtures of ethers. V. Diisopropyl ether or oxolane with 2- or 3-chloroanilines at 303.15, 313.15 and 323.15 K:	https://www.doi.org/10.1016/j.tca.2011.07.005
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1287.mol

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation

hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion 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
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
speedsl:	Speed of sound in fluid
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume