

o-Chloroaniline

Other names:	1-Amino-2-chlorobenzene
	2-CHLORO-BENZENAMINE
	2-Chloroaniline
	2-Chlorobenzenamine
	2-Chlorophenylamine
	2-chlorobenzamine
	2-chlorobenzeneamine
	Aniline, o-chloro-
	Azoic diazo component 44, base
	Benzenamine, 2-chloro-
	Benzeneamine, 2-chloro-
	Fast Yellow GC Base
	NSC 6183
	O-AMINOCHLOROBENZENE
	o-Chloraniline
	o-Chloroaminobenzene
Inchi:	InChI=1S/C6H6ClN/c7-5-3-1-2-4-6(5)8/h1-4H,8H2
InchiKey:	AKCRQHGGQIJBRMN-UHFFFAOYSA-N
Formula:	C6H6ClN
SMILES:	Nc1ccccc1Cl
Mol. weight [g/mol]:	127.57
CAS:	95-51-2

Physical Properties

Property code	Value	Unit	Source
chl	-3237.50 ± 1.40	kJ/mol	NIST Webbook
gf	156.94	kJ/mol	Joback Method
hf	75.94	kJ/mol	Joback Method
hfl	-4.64	kJ/mol	NIST Webbook
hfus	12.38	kJ/mol	Heat Capacities of Chloroanilines and Chloronitrobenzenes
hvap	56.40 ± 1.60	kJ/mol	NIST Webbook
hvap	57.10 ± 0.50	kJ/mol	NIST Webbook
ie	8.50	eV	NIST Webbook
ie	7.90	eV	NIST Webbook
log10ws	-1.52		Estimated Solubility Method

log10ws	-1.52		Aqueous Solubility Prediction Method
logp	1.922		Crippen Method
mcvol	93.860	ml/mol	McGowan Method
pc	4704.19	kPa	Joback Method
rinpol	1094.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1092.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1095.00		NIST Webbook
rinpol	1092.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1125.00		NIST Webbook
rinpol	1095.40		NIST Webbook
ripol	1879.00		NIST Webbook
ripol	1879.00		NIST Webbook
ripol	1879.00		NIST Webbook
ripol	1901.00		NIST Webbook
tb	481.99 ± 0.07	K	NIST Webbook
tb	482.15 ± 1.00	K	NIST Webbook
tb	482.00	K	NIST Webbook
tb	480.15	K	KDB
tb	480.20 ± 2.00	K	NIST Webbook
tc	716.47	K	Joback Method
tf	271.05 ± 0.10	K	NIST Webbook
tf	264.90	K	Aqueous Solubility Prediction Method
tf	269.65 ± 0.50	K	NIST Webbook
tf	271.21 ± 0.05	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	205.09	J/mol×K	637.08	Joback Method
cpg	212.01	J/mol×K	676.77	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
cpg	218.41	J/mol×K	716.47	Joback Method
hfust	12.38	kJ/mol	269.20	NIST Webbook
hfust	8.81	kJ/mol	271.00	NIST Webbook
hvapt	50.70	kJ/mol	439.50	NIST Webbook
hvapt	57.10 ± 1.00	kJ/mol	312.00	NIST Webbook
hvapt	58.20 ± 1.40	kJ/mol	311.50	NIST Webbook
rho1	1183.26	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
rho1	1192.97	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
rho1	1187.92	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

rhoI	1202.38	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
rhoI	1197.56	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
speedsl	1402.00	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	1438.00	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	1470.00	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

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.50330e+01
Coeff. B	-4.32789e+03
Coeff. C	-6.64440e+01
Temperature range (K), min.	359.95
Temperature range (K), max.	511.63

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$
Coeff. A	1.36416e+02
Coeff. B	-1.19812e+04
Coeff. C	-1.76606e+01
Coeff. D	9.33757e-06
Temperature range (K), min.	271.05
Temperature range (K), max.	722.00

Sources

Heat Capacities of Chloroanilines and Chloronitrobenzenes: Study on thermo physical properties of binary mixture containing aromatic alcohols with aromatic substituted alcohols. <https://www.doi.org/10.1021/je700080k>

Thermodynamic and acoustic properties of binary mixtures of ethers. <https://www.doi.org/10.1016/j.fluid.2018.01.025>

NIST Webbook. <https://www.doi.org/10.1016/j.tca.2011.07.005>

on 2-chloroanilines at 603.15, 613.15 and 323.15 K. <http://webbook.nist.gov/cgi/cbook.cgi?ID=C95512&Units=SI>

Joback Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

KDB: <https://www.thermo.com/files/research/kdb/mol/mol1286.mol>

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

McGowan Method: https://en.wikipedia.org/wiki/Joback_method

KDB Vapor Pressure Data: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1286>

The Yaws Handbook of Vapor Pressure: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas 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
rho:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
speedsl:	Speed of sound in fluid
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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