Benzenamine, 3,4-dichloro-

Other names:	1-Amino-3,4-dichlorobenzene
	3,4-DCA
	3,4-DICHLOROBENZENEAMINE
	3,4-Dichloranilin
	3,4-Dichloraniline
	3,4-Dichloroaniline
	3,4-Dichlorobenzenamine
	3,4-Dichlorophenylamine
	4,5-DICHLOROANILINE
	4-Amino-1,2-dichlorobenzene
	Aniline, 3,4-dichloro-
	DCA
	LY 004892
	NSC 247
Inchi:	InChI=1S/C6H5Cl2N/c7-5-2-1-4(9)3-6(5)8/h1-3H,9H2
InchiKey:	SDYWXFYBZPNOFX-UHFFFAOYSA-N
Formula:	C6H5Cl2N
SMILES:	Nc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]:	162.02
CAS:	95-76-1

Physical Properties

Property code	Value	Unit	Source
chs	-3033.80 ± 2.20	kJ/mol	NIST Webbook
gf	135.38	kJ/mol	Joback Method
hf	48.73	kJ/mol	Joback Method
hfs	-89.12	kJ/mol	NIST Webbook
hfus	18.15	kJ/mol	Joback Method
hvap	51.96	kJ/mol	Joback Method
log10ws	-3.24		Aqueous Solubility Prediction Method
logp	2.576		Crippen Method
mcvol	106.100	ml/mol	McGowan Method
pc	4385.77	kPa	Joback Method
rinpol	1377.00		NIST Webbook
rinpol	1387.00		NIST Webbook
rinpol	1373.00		NIST Webbook

rinpol	1377.00		NIST Webbook
rinpol	1372.00		NIST Webbook
rinpol	1387.00		NIST Webbook
rinpol	1373.00		NIST Webbook
ripol	2519.00		NIST Webbook
ripol	2519.00		NIST Webbook
ripol	2519.00		NIST Webbook
tb	545.20	K	NIST Webbook
tc	765.61	K	Joback Method
tf	345.30 ± 0.10	K	NIST Webbook
tf	345.14 ± 0.20	K	NIST Webbook
tf	618.10 ± 0.20	K	NIST Webbook
vc	0.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.63	J/mol×K	520.71	Joback Method
cpg	199.84	J/mol×K	561.53	Joback Method
cpg	207.47	J/mol×K	602.34	Joback Method
cpg	214.54	J/mol×K	643.16	Joback Method
cpg	221.09	J/mol×K	683.97	Joback Method
cpg	227.13	J/mol×K	724.79	Joback Method
cpg	232.70	J/mol×K	765.61	Joback Method
hfust	21.69	kJ/mol	344.50	NIST Webbook
hvapt	58.60	kJ/mol	482.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	418.20	K	2.00	NIST Webbook

Correlations

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50249e+01
Coeff. B	-4.81734e+03
Coeff. C	-8.22860e+01
Temperature range (K), min.	409.17
Temperature range (K), max.	578.23

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.61445e+01
Coeff. B	-1.17125e+04
Coeff. C	-1.12823e+01
Coeff. D	3.47347e-06
Temperature range (K), min.	344.65
Temperature range (K), max.	800.00

Sources

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=1798
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
KDB: https://www.cheric.org/files/research/kdb/mol/mol1798.mol
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C95761&Units=SI

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas 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
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume