Benzenamine, 3,5-dichloro-

Other names:	3,5-dichloroaminobenzene
	3,5-dichloroaniline
	aniline, 3,5-dichloro-
Inchi:	InChI=1S/C6H5Cl2N/c7-4-1-5(8)3-6(9)2-4/h1-3H,9H2
InchiKey:	UQRLKWGPEVNVHT-UHFFFAOYSA-N
Formula:	C6H5Cl2N
SMILES:	Nc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]:	162.02
CAS:	626-43-7

Physical Properties

Property code	Value	Unit	Source
gf	135.38	kJ/mol	Joback Method
hf	48.73	kJ/mol	Joback Method
hfus	18.15	kJ/mol	Joback Method
hvap	51.96	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.576		Crippen Method
mcvol	106.100	ml/mol	McGowan Method
pc	4385.77	kPa	Joback Method
rinpol	1352.00		NIST Webbook
rinpol	1347.00		NIST Webbook
rinpol	1349.00		NIST Webbook
ripol	2469.00		NIST Webbook
ripol	2469.00		NIST Webbook
tb	532.00 ± 1.00	K	NIST Webbook
tc	765.61	K	Joback Method
tf	323.16	K	Determination and thermodynamic modeling of solid-liquid phase equilibrium for 3,5-dichloroaniline in pure solvents and ternary 3,5-dichloroaniline + 1,3,5-trichlorobenzene + toluene system
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
pvap	29.60	kPa	484.05	Measurement and Correlation of the Vapor Pressure of 3,5-Dichloroaniline
pvap	12.95	kPa	453.88	Measurement and Correlation of the Vapor Pressure of 3,5-Dichloroaniline
pvap	14.44	kPa	457.69	Measurement and Correlation of the Vapor Pressure of 3,5-Dichloroaniline
pvap	16.64	kPa	463.14	Measurement and Correlation of the Vapor Pressure of 3,5-Dichloroaniline
pvap	17.20	kPa	464.40	Measurement and Correlation of the Vapor Pressure of 3,5-Dichloroaniline
pvap	18.21	kPa	466.41	Measurement and Correlation of the Vapor Pressure of 3,5-Dichloroaniline
pvap	19.57	kPa	468.53	Measurement and Correlation of the Vapor Pressure of 3,5-Dichloroaniline
pvap	19.87	kPa	469.09	Measurement and Correlation of the Vapor Pressure of 3,5-Dichloroaniline

pvap	20.20	kPa	470.18	Measurement and Correlation of the Vapor Pressure of 3,5-Dichloroaniline
pvap	22.16	kPa	473.66	Measurement and Correlation of the Vapor Pressure of 3,5-Dichloroaniline
pvap	23.01	kPa	474.48	Measurement and Correlation of the Vapor Pressure of 3,5-Dichloroaniline
pvap	23.48	kPa	475.29	Measurement and Correlation of the Vapor Pressure of 3,5-Dichloroaniline
pvap	24.67	kPa	477.65	Measurement and Correlation of the Vapor Pressure of 3,5-Dichloroaniline
pvap	27.19	kPa	481.31	Measurement and Correlation of the Vapor Pressure of 3,5-Dichloroaniline
pvap	10.25	kPa	446.60	Measurement and Correlation of the Vapor Pressure of 3,5-Dichloroaniline
pvap	32.05	kPa	487.88	Measurement and Correlation of the Vapor Pressure of 3,5-Dichloroaniline
pvap	35.09	kPa	490.85	Measurement and Correlation of the Vapor Pressure of 3,5-Dichloroaniline
pvap	36.63	kPa	492.54	Measurement and Correlation of the Vapor Pressure of 3,5-Dichloroaniline
pvap	38.71	kPa	495.30	Measurement and Correlation of the Vapor Pressure of 3,5-Dichloroaniline
pvap	41.11	kPa	497.31	Measurement and Correlation of the Vapor Pressure of 3,5-Dichloroaniline

pvap	44.06	kPa	500.72	Measurement and Correlation of the Vapor Pressure of 3,5-Dichloroaniline
pvap	47.64	kPa	503.96	Measurement and Correlation of the Vapor Pressure of 3,5-Dichloroaniline
pvap	51.52	kPa	507.34	Measurement and Correlation of the Vapor Pressure of 3,5-Dichloroaniline
pvap	55.17	kPa	509.76	Measurement and Correlation of the Vapor Pressure of 3,5-Dichloroaniline
pvap	58.05	kPa	512.08	Measurement and Correlation of the Vapor Pressure of 3,5-Dichloroaniline
pvap	60.01	kPa	513.94	Measurement and Correlation of the Vapor Pressure of 3,5-Dichloroaniline
pvap	63.13	kPa	516.09	Measurement and Correlation of the Vapor Pressure of 3,5-Dichloroaniline
pvap	66.66	kPa	518.15	Measurement and Correlation of the Vapor Pressure of 3,5-Dichloroaniline
pvap	68.55	kPa	519.82	Measurement and Correlation of the Vapor Pressure of 3,5-Dichloroaniline
pvap	71.60	kPa	521.75	Measurement and Correlation of the Vapor Pressure of 3,5-Dichloroaniline
pvap	75.31	kPa	523.61	Measurement and Correlation of the Vapor Pressure of 3,5-Dichloroaniline
pvap	78.65	kPa	525.72	Measurement and Correlation of the Vapor Pressure of 3,5-Dichloroaniline

pvap	82.54	kPa	528.31	Measurement and Correlation of the Vapor Pressure of 3,5-Dichloroaniline
pvap	87.17	kPa	530.51	Measurement and Correlation of the Vapor Pressure of 3,5-Dichloroaniline
pvap	91.08	kPa	532.90	Measurement and Correlation of the Vapor Pressure of 3,5-Dichloroaniline
pvap	95.84	kPa	534.94	Measurement and Correlation of the Vapor Pressure of 3,5-Dichloroaniline

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	533.20	K	98.80	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Determination and thermodynamic modeling of solid-liquid phase equilibrium for 3,5-dichloroaniline in pure solvents and ternary https://www.doi.org/10.1016/j.jct.2016.03.007

Measurement and Correlation of the Vapor Pressure of 3,5-Dichloroaniline: https://www.doi.org/10.1021/je3013638

Solubility Measurement and Correlation for 3,5-Dichloroaniline in (Methanol + 1,3,5-Trichlorobenzene + Toluene or Hexane) and (Ethanol + Water) Mixed Solvents: https://www.doi.org/10.1021/je500744k

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=C626437&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
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