Benzenamine, 2,4,6-trichloro-

Other names:	1-Amino-2,4,6-trichlorobenzene
	2,4,6-Trichloroaniline
	2,4,6-Trichlorobenzenamine
	2,4,6-Trichlorophenylamine
	Aniline, 2,4,6-trichloro-
	s-Trichloroaniline
	sym-Trichloroaniline
Inchi:	InChI=1S/C6H4Cl3N/c7-3-1-4(8)6(10)5(9)2-3/h1-2H,10H2
InchiKey:	NATVSFWWYVJTAZ-UHFFFAOYSA-N
Formula:	C6H4Cl3N
SMILES:	Nc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]:	196.46
CAS:	634-93-5

Physical Properties

Property code	Value	Unit	Source
gf	113.82	kJ/mol	Joback Method
hf	21.52	kJ/mol	Joback Method
hfus	21.96	kJ/mol	Joback Method
hsub	85.30 ± 1.90	kJ/mol	NIST Webbook
hvap	57.01	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	3.229		Crippen Method
mcvol	118.340	ml/mol	McGowan Method
pc	4098.62	kPa	Joback Method
rinpol	1367.00		NIST Webbook
rinpol	1379.00		NIST Webbook
rinpol	1367.00		NIST Webbook
rinpol	1362.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1367.00		NIST Webbook
rinpol	1398.00		NIST Webbook
tb	535.20	K	NIST Webbook
tc	813.61	K	Joback Method
tf	394.38	K	Joback Method
vc	0.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.50	J/mol×K	771.86	Joback Method
cpg	209.61	J/mol×K	563.12	Joback Method
cpg	216.78	J/mol×K	604.87	Joback Method
cpg	223.43	J/mol×K	646.62	Joback Method
cpg	229.59	J/mol×K	688.36	Joback Method
cpg	235.27	J/mol×K	730.11	Joback Method
cpg	245.30	J/mol×K	813.61	Joback Method
hvapt	92.90	kJ/mol	471.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	535.20	K	99.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.55173e+01
Coeff. B	-1.11949e+04
Coeff. C	4.70000e-01
Temperature range (K), min.	407.00
Temperature range (K), max.	553.58

Sources

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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C634935&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
hsub:	Enthalpy of sublimation at standard conditions
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume