Benzenamine, 2,3,4-trichloro-

Other names: Aniline, 2,3,4-trichloro-
2,3,4-Trichloroaniline
Inchi: InChI=1S/C6H4Cl3N/c7-3-1-2-4(10)6(9)5(3)8/h1-2H,10H2
InchiKey: RRJUYQOFOMFVQS-UHFFFAOYSA-N
Formula: C6H4Cl3N
SMILES: Nc1ccc(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 196.46
CAS: 634-67-3

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
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
tb	563.12	K	Joback Method
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	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	240.50	J/mol×K	771.86	Joback Method
cpg	245.30	J/mol×K	813.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C634673&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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