Benzenamine, 2,3-dichloro-

Other names: Aniline, 2,3-dichloro-
2,3-Dichloroaniline
Inchi: InChI=1S/C6H5Cl2N/c7-4-2-1-3-5(9)6(4)8/h1-3H,9H2
InchiKey: BRPSAOUFIJSKOT-UHFFFAOYSA-N
Formula: C6H5Cl2N
SMILES: Nc1cccc(Cl)c1Cl
Mol. weight [g/mol]: 162.02
CAS: 608-27-5

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
tb	520.71	K	Joback Method
tc	765.61	K	Joback Method
tf	351.94	K	Joback Method
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

Sources

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=C608275&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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