5-Chloro-1,3-phenylenediamine

Other names:	3,5-Diaminochlorobenzene
	5-Chloro-m-phenylenediamine
	1,3-Benzenediamine, 5-chloro-
	5-Chloro-1,3-benzenediamine
Inchi:	InChI=1S/C6H7ClN2/c7-4-1-5(8)3-6(9)2-4/h1-3H,8-9H2
InchiKey:	VZNUCJOYPXKLTA-UHFFFAOYSA-N
Formula:	C6H7ClN2
SMILES:	Nc1cc(N)cc(Cl)c1
Mol. weight [g/mol]:	142.59
CAS:	33786-89-9

Physical Properties

Property code	Value	Unit	Source
gf	213.76	kJ/mol	Joback Method
hf	98.26	kJ/mol	Joback Method
hfus	19.15	kJ/mol	Joback Method
hvap	58.22	kJ/mol	Joback Method
log10ws	-1.42		Crippen Method
logp	1.504		Crippen Method
mcvol	103.840	ml/mol	McGowan Method
pc	4987.39	kPa	Joback Method
tb	555.81	K	Joback Method
tc	805.36	K	Joback Method
tf	405.28	K	Joback Method
vc	0.370	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.19	J/mol×K	555.81	Joback Method
cpg	225.31	J/mol×K	597.40	Joback Method
cpg	233.79	J/mol×K	638.99	Joback Method
cpg	241.64	J/mol×K	680.58	Joback Method
cpg	248.91	J/mol×K	722.17	Joback Method

cpg	255.62	J/mol×K	763.77	Joback Method
cpg	261.79	J/mol×K	805.36	Joback Method

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=C33786899&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume