1,3-Benzenediamine, 4-chloro-

Other names:	m-Phenylenediamine, 4-chloro-
	C.I. 76027
	1-Chloro-2,4-Diaminobenzene
	4-Chloro-m-phenylenediamine
	4-Chloro-1,3-benzenediamine
	4-Chloro-1,3-phenylenediamine
	NCI-C03305
	4-Chloro-meta-phenylenediamine
	4-Chlorophene-1,3-diamine
	4-Chlorophenylene-1,3-diamine
	p-Chlor-m-fenylendiamin
	p-Chloro-m-phenylenediamine
	4-Cl-m-Pd
	3-Amino-4-chloroaniline
	NSC 6074
	4-chlorobenzene-1,3-diamine
	2,4-Diaminochlorobenzene
Inchi:	InChI=1S/C6H7ClN2/c7-5-2-1-4(8)3-6(5)9/h1-3H,8-9H2
InchiKey:	ZWUBBMDHSZDNTA-UHFFFAOYSA-N
Formula:	C6H7ClN2
SMILES:	Nc1ccc(Cl)c(N)c1
Mol. weight [g/mol]:	142.59
CAS:	5131-60-2

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=C5131602&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