Benzenamine, 3-chloro-4-methyl-

Other names:	p-Toluidine, 3-chloro-
	DRC 1347
	1-Amino-3-Chloro-4-methylbenzene
	2-Chloro-4-aminotoluene
	3-Chloro-p-toluidine
	3-Chloro-4-methylaniline
	3-Chloro-4-methylbenzenamine
	4-Methyl-3-chloroaniline
	3-Chloro-4-toluidine
	4-Amino-2-chlorotoluene
	DRC 1339
	NCI-C02040
	3-Chloro-4-methylphenylamine
	NSC 96620
	2-chloro-4-toluidine
Inchi:	InChI=1S/C7H8ClN/c1-5-2-3-6(9)4-7(5)8/h2-4H,9H2,1H3
InchiKey:	RQKFYFNZSHWXAW-UHFFFAOYSA-N
Formula:	C7H8ClN
SMILES:	Cc1ccc(N)cc1Cl
Mol. weight [g/mol]:	141.60
CAS:	95-74-9

Physical Properties

Property code	Value	Unit	Source
chl	-3607.00 ± 6.70	kJ/mol	NIST Webbook
gf	155.73	kJ/mol	Joback Method
hf	75.30 ± 7.10	kJ/mol	NIST Webbook
hfl	23.00 ± 6.70	kJ/mol	NIST Webbook
hfus	16.54	kJ/mol	Joback Method
hvap	49.80	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	2.231		Crippen Method
mcvol	107.950	ml/mol	McGowan Method
pc	4062.13	kPa	Joback Method
rinpol	1257.30		NIST Webbook
rinpol	1257.30		NIST Webbook
ripol	1957.00		NIST Webbook

ripol	1957.00		NIST Webbook
ripol	1957.00		NIST Webbook
tb	510.70	K	NIST Webbook
tc	741.33	K	Joback Method
tf	333.29	K	Joback Method
vc	0.398	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	211.08	J/mol×K	506.16	Joback Method
cpg	221.33	J/mol×K	545.35	Joback Method
cpg	230.94	J/mol×K	584.55	Joback Method
cpg	239.95	J/mol×K	623.74	Joback Method
cpg	248.37	J/mol×K	662.94	Joback Method
cpg	256.22	J/mol×K	702.13	Joback Method
cpg	263.54	J/mol×K	741.33	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C95749&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase 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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume