

2-Chloro-5-methylaniline

Other names:	Benzenamine, 2-chloro-5-methyl-6-chloro-m-toluidine
Inchi:	InChI=1S/C7H8ClN/c1-5-2-3-6(8)7(9)4-5/h2-4H,9H2,1H3
InchiKey:	HPSCXFOQUFPEPE-UHFFFAOYSA-N
Formula:	C7H8ClN
SMILES:	<chem>Cc1ccc(Cl)c(N)c1</chem>
Mol. weight [g/mol]:	141.60
CAS:	95-81-8

Physical Properties

Property code	Value	Unit	Source
gf	155.73	kJ/mol	Joback Method
hf	43.83	kJ/mol	Joback Method
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	1201.00		NIST Webbook
rinpol	1201.00		NIST Webbook
ripol	1975.00		NIST Webbook
ripol	1975.00		NIST Webbook
tb	502.20	K	NIST Webbook
tc	741.33	K	Joback Method
tf	333.29	K	Joback Method
vc	0.398	m ³ /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

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=C95818&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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

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