

Benzenamine, 4-chloro-2-methyl-

Other names:	o-Toluidine, 4-chloro- p-Chloro-o-toluidine Daito Red Base TR Fast Red Base TR Fast Red TR Base Fast Red TRO Base Fast Red 5CT Base Kako Red TR Base Mitsui Red TR Base Red Base NTR Red TR base Sanyo Fast Red TR Base 2-Amino-5-chlorotoluene 2-Methyl-4-chloroaniline 4-Chloro-o-toluidine 4-Chloro-2-methylaniline 4-Chloro-2-methylbenzeneamine 4-Chloro-2-toluidine 4-Chloro-6-methylaniline Amarthol Fast Red TR Base Azoene Fast Red TR Base Azoic diazo component 11, base Brentamine Fast Red TR Base Deval Red K Deval Red TR Diazo Fast Red TRA Fast Red TR11 Fast Red TR Kambamine Red TR Red Base Ciba IX Red Base Irga IX Tulabase Fast Red TR 3-Chloro-6-aminotoluene 5-Chloro-2-aminotoluene Fast Red TR-T Base NSC 4979
Inchi:	InChI=1S/C7H8ClN/c1-5-4-6(8)2-3-7(5)9/h2-4H,9H2,1H3
InchiKey:	CXNVOWPRHWWCQR-UHFFFAOYSA-N
Formula:	C7H8ClN
SMILES:	Cc1cc(Cl)ccc1N

Mol. weight [g/mol]: 141.60
CAS: 95-69-2

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	1247.30		NIST Webbook
rinpol	1256.00		NIST Webbook
rinpol	1256.00		NIST Webbook
ripol	2155.00		NIST Webbook
ripol	2155.00		NIST Webbook
tb	514.20	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=C95692&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	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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