Benzenamine, 3-chloro-2-methyl-

Other names:	o-Toluidine, 3-chloro-
	o-Methyl-m-chloroaniline
	Fast Scarlet TR base
	Scarlet TR base
	3-Chloro-o-toluidine
	3-Chloro-2-methylphenylamine
	3-Chloro-2-toluidine
	6-Chloro-2-aminotoluene
	3-Chloro-2-methylaniline
	2-Amino-6-chlorotoluene
	Azoic diazo component 46
	1-Amino-3-chloro-2-methylbenzene
	3-Chlor-2-toluidin
	1-Amino-2-chloro-6-methylbenzene
	2-Methyl-3-chloroaniline
	6-Chloro-2-amino-1-methylbenzene
	NSC 6184
Inchi:	InChI=1S/C7H8ClN/c1-5-6(8)3-2-4-7(5)9/h2-4H,9H2,1H3
InchiKey:	ZUVPLKVDZNDZCM-UHFFFAOYSA-N
Formula:	C7H8ClN
SMILES:	Cc1c(N)cccc1Cl
Mol. weight [g/mol]:	141.60
CAS:	87-60-5

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	1182.00		NIST Webbook
rinpol	1182.00		NIST Webbook
ripol	1893.00		NIST Webbook

ripol	1893.00		NIST Webbook
ripol	1893.00		NIST Webbook
tb	518.20	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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	389.20	K	1.30	NIST Webbook

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=C87605&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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

https://www.chemeo.com/cid/51-469-5/Benzenamine-3-chloro-2-methyl.pdf

Generated by Cheméo on 2024-10-12 07:42:59.757599518 +0000 UTC m=+3299842.394568765.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.