2-CHLORO-P-TOLUIDINE

Other names:	p-Toluidine, 2-chloro-
	2-Chloro-p-toluidine
	2-Chloro-4-methylaniline
	4-Amino-3-chlorotoluene
	2-Chlor-4-toluidin
	4-Methyl-2-chloroaniline
	2-Chloro-4-methylbenzamine
	3-Chloro-4-aminotoluene
	NSC 60120
Inchi:	InChI=1S/C7H8ClN/c1-5-2-3-7(9)6(8)4-5/h2-4H,9H2,1H3
InchiKey:	XGYLSRFSXKAYCR-UHFFFAOYSA-N
Formula:	C7H8ClN
SMILES:	Cc1ccc(N)c(Cl)c1
Mol. weight [g/mol]:	141.60

Physical Properties

Property code	Value	Unit	Source
af	0.4513		Cheméo Relay (1.0)
hf	10.64	kJ/mol	Cheméo Relay (1.0)
hfus	16.54	kJ/mol	Joback Method
hvap	59.15	kJ/mol	Cheméo Relay (1.0)
ie	7.78	eV	Cheméo Relay (1.0)
log10ws	-2.03		Cheméo Relay (1.0)
logp	2.231		Crippen Method
mcvol	107.950	ml/mol	McGowan Method
pc	4062.13	kPa	Joback Method
rinpol	1195.00		NIST Webbook
rinpol	1195.00		NIST Webbook
rinpol	1197.10		NIST Webbook
ripol	2160.00		NIST Webbook
ripol	2160.00		NIST Webbook
tb	497.20	K	NIST Webbook
tc	748.80	K	Cheméo Relay (1.0)
tf	313.95	K	Cheméo Relay (1.0)

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	492.20	K	97.60	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C615656&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor

cpg: Ideal gas heat capacity

hf: Enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

hvap: Enthalpy of vaporization at standard conditions

ie:	Ionization energy
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