Phenol, 4-chloro-3-methyl-

Other names:	1-Chloro-2-methyl-4-hydroxybenzene
	2-Chloro-5-hydroxytoluene
	2-Chloro-hydroxytoluene
	3-Methyl-4-chlorophenol
	4-Chloro-3-cresol
	4-Chloro-3-methylphenol
	4-Chloro-5-methylphenol
	4-Chloro-m-cresol
	6-Chloro-3-hydroxytoluene
	Aptal
	Baktol
	Baktolan
	CMK
	Candaseptic
	Chlorocresol
	Lysochlor
	NSC 4166
	Ottafact
	PCMC
	Parmetol
	Parol
	Peritonan
	Phenol, 4-chloro-5-methyl-
	Preventol CMK
	Raschit
	Raschit K
	Rasen-Anicon
	Rcra waste number U039
	m-Cresol, 4-chloro-
	p-Chlor-m-cresol
	p-Chloro-m-cresol
	p-Chlorocresol
	para-Chloro-meta-cresol
Inchi:	InChI=1S/C7H7ClO/c1-5-4-6(9)2-3-7(5)8/h2-4,9H,1H3
InchiKey:	CFKMVGJGLGKFKI-UHFFFAOYSA-N
Formula:	C7H7ClO
SMILES:	Cc1cc(O)ccc1Cl
Mol. weight [g/mol]:	142.58
CAS:	59-50-7

Physical Properties

Property code	Value	Unit	Source
gf	-55.71	kJ/mol	Joback Method
hf	-155.80	kJ/mol	Joback Method
hfus	17.52	kJ/mol	Joback Method
hvap	51.51	kJ/mol	Joback Method
log10ws	-1.57		Aqueous Solubility Prediction Method
logp	2.354		Crippen Method
mcvol	103.840	ml/mol	McGowan Method
pc	4678.49	kPa	Joback Method
rinpol	1258.00		NIST Webbook
rinpol	1294.00		NIST Webbook
rinpol	1297.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	218.50		NIST Webbook
rinpol	220.20		NIST Webbook
rinpol	1297.30		NIST Webbook
rinpol	1291.00		NIST Webbook
rinpol	1280.00		NIST Webbook
rinpol	1277.00		NIST Webbook
rinpol	1260.10		NIST Webbook
rinpol	1293.00		NIST Webbook
rinpol	1283.00		NIST Webbook
rinpol	1283.00		NIST Webbook
ripol	2508.93		NIST Webbook
ripol	2517.86		NIST Webbook
ripol	2522.35		NIST Webbook
ripol	2509.04		NIST Webbook
tb	505.00 ± 6.00	K	NIST Webbook
tb	508.20	K	NIST Webbook
tc	746.12	K	Joback Method
tf	339.90	K	Aqueous Solubility Prediction Method
tf	328.70 ± 2.00	K	NIST Webbook
vc	0.335	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.51	J/mol×K	509.27	Joback Method
cpg	246.99	J/mol×K	706.65	Joback Method
cpg	240.10	J/mol×K	667.17	Joback Method
cpg	232.68	J/mol×K	627.70	Joback Method
cpg	224.67	J/mol×K	588.22	Joback Method
cpg	215.97	J/mol×K	548.75	Joback Method
cpg	253.43	J/mol×K	746.12	Joback Method
dvisc	0.0000896	Pa×s	509.27	Joback Method
dvisc	0.0001330	Pa×s	482.60	Joback Method
dvisc	0.0002067	Pa×s	455.92	Joback Method
dvisc	0.0003392	Pa×s	429.25	Joback Method
dvisc	0.0005946	Pa×s	402.58	Joback Method
dvisc	0.0011285	Pa×s	375.90	Joback Method
dvisc	0.0023623	Pa×s	349.23	Joback Method

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C59507&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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