5-Chloro-2-methylphenol

Other names:	2-Methyl-5-chlorophenol
	3-Chloro-6-methylphenol
	5-Chloro-2-methylphenol
	5-Chloro-o-cresol
	o-Cresol, 5-chloro-
Inchi:	InChI=1S/C7H7ClO/c1-5-2-3-6(8)4-7(5)9/h2-4,9H,1H3
InchiKey:	KKFPXGXMSBBNJI-UHFFFAOYSA-N
Formula:	C7H7ClO
SMILES:	Cc1ccc(Cl)cc1O
Mol. weight [g/mol]:	142.59

Physical Properties

Property code	Value	Unit	Source
af	0.4872		Cheméo Relay (1.0)
gf	-55.71	kJ/mol	Joback Method
hf	-156.71	kJ/mol	Cheméo Relay (1.0)
hfus	17.52	kJ/mol	Joback Method
hvap	68.14	kJ/mol	Cheméo Relay (1.0)
ie	8.45	eV	Cheméo Relay (1.0)
log10ws	-1.49		Cheméo Relay (1.0)
logp	2.354		Crippen Method
mcvol	103.840	ml/mol	McGowan Method
pc	4678.49	kPa	Joback Method
tb	493.00	K	Cheméo Relay (1.0)
tc	726.06	K	Cheméo Relay (1.0)
tf	333.15	K	Cheméo Relay (1.0)
vc	0.358	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.51	J/mol×K	509.27	Joback Method
cpg	215.97	J/mol×K	548.75	Joback Method
cpg	224.67	J/mol×K	588.22	Joback Method

cpg	232.68	J/mol×K	627.70	Joback Method
cpg	240.10	J/mol×K	667.17	Joback Method
cpg	246.99	J/mol×K	706.65	Joback Method
cpg	253.43	J/mol×K	746.12	Joback Method
dvisc	0.0023623	Pa×s	349.23	Joback Method
dvisc	0.0011285	Pa×s	375.90	Joback Method
dvisc	0.0005946	Pa×s	402.58	Joback Method
dvisc	0.0003392	Pa×s	429.25	Joback Method
dvisc	0.0002067	Pa×s	455.92	Joback Method
dvisc	0.0001330	Pa×s	482.60	Joback Method
dvisc	0.0000896	Pa×s	509.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5306989&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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume