Phenol, 2-chloro-4-methoxy-

Other names: 2-Chloro-4-methoxyphenol
Inchi: InChI=1S/C7H7ClO2/c1-10-5-2-3-7(9)6(8)4-5/h2-4,9H,1H3
InchiKey: GNVRRKLFFYSLGT-UHFFFAOYSA-N
Formula: C7H7ClO2
SMILES: COc1ccc(O)c(Cl)c1
Mol. weight [g/mol]: 158.58
CAS: 18113-03-6

Physical Properties

Property code	Value	Unit	Source
gf	-160.71	kJ/mol	Joback Method
hf	-288.02	kJ/mol	Joback Method
hfus	18.71	kJ/mol	Joback Method
hvap	53.92	kJ/mol	Joback Method
log10ws	-1.82		Crippen Method
logp	2.054		Crippen Method
mcvol	109.710	ml/mol	McGowan Method
pc	4571.55	kPa	Joback Method
rinpol	1260.10		NIST Webbook
tb	531.69	K	Joback Method
tc	765.48	K	Joback Method
tf	371.46	K	Joback Method
vc	0.352	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.02	J/mol×K	531.69	Joback Method
cpg	236.28	J/mol×K	570.65	Joback Method
cpg	244.90	J/mol×K	609.62	Joback Method
cpg	252.93	J/mol×K	648.58	Joback Method
cpg	260.42	J/mol×K	687.55	Joback Method
cpg	267.44	J/mol×K	726.51	Joback Method
cpg	274.04	J/mol×K	765.48	Joback Method

dvisc	0.0013306	Pa×s	371.46	Joback Method
dvisc	0.0006751	Pa×s	398.17	Joback Method
dvisc	0.0003730	Pa×s	424.87	Joback Method
dvisc	0.0002211	Pa×s	451.58	Joback Method
dvisc	0.0001389	Pa×s	478.28	Joback Method
dvisc	0.0000917	Pa×s	504.99	Joback Method
dvisc	0.0000631	Pa×s	531.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18113036&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume