Phenol, 4-chloro-5-methyl-2-(1-methylethyl)-

Other names:	Thymol, 6-chloro-
	Chlorothymol
	Chlorthymol
	4-Chloro-2-isopropyl-5-methylphenol
	4-Chlorothymol
	4-Chloro-6-isopropyl-3-methylphenol
	6-chlorothymol
Inchi:	InChI=1S/C10H13ClO/c1-6(2)8-5-9(11)7(3)4-10(8)12/h4-6,12H,1-3H3
InchiKey:	KFZXVMNBUMVKLN-UHFFFAOYSA-N
Formula:	C10H13ClO
SMILES:	Cc1cc(O)c(C(C)C)cc1Cl
Mol. weight [g/mol]:	184.66
CAS:	89-68-9

Physical Properties

Property code	Value	Unit	Source
gf	-42.52	kJ/mol	Joback Method
hf	-234.47	kJ/mol	Joback Method
hfus	21.38	kJ/mol	Joback Method
hvap	58.47	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	3.477		Crippen Method
mcvol	146.110	ml/mol	McGowan Method
pc	3239.34	kPa	Joback Method
rinpol	1486.00		NIST Webbook
tb	582.45	K	Joback Method
tc	812.18	K	Joback Method
tf	380.56	K	Joback Method
vc	0.496	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.46	J/mol×K	582.45	Joback Method

cpg	349.05	J/mol×K	620.74	Joback Method
cpg	360.82	J/mol×K	659.03	Joback Method
cpg	371.86	J/mol×K	697.32	Joback Method
cpg	382.23	J/mol×K	735.61	Joback Method
cpg	392.01	J/mol×K	773.90	Joback Method
cpg	401.28	J/mol×K	812.18	Joback Method
dvisc	0.0013925	Pa×s	380.56	Joback Method
dvisc	0.0006051	Pa×s	414.21	Joback Method
dvisc	0.0002980	Pa×s	447.86	Joback Method
dvisc	0.0001620	Pa×s	481.50	Joback Method
dvisc	0.0000954	Pa×s	515.15	Joback Method
dvisc	0.0000599	Pa×s	548.80	Joback Method
dvisc	0.0000397	Pa×s	582.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C89689&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

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