Phenol, 2-chloro-4-ethyl-

Other names: 2-chloro-4-ethylphenol
Inchi: InChI=1S/C8H9ClO/c1-2-6-3-4-8(10)7(9)5-6/h3-5,10H,2H2,1H3
InchiKey: QNQRRCHRJHMSLF-UHFFFAOYSA-N
Formula: C8H9ClO
SMILES: CCc1ccc(O)c(Cl)c1
Mol. weight [g/mol]: 156.61
CAS: 18980-00-2

Physical Properties

Property code	Value	Unit	Source
gf	-47.29	kJ/mol	Joback Method
hf	-176.44	kJ/mol	Joback Method
hfus	20.11	kJ/mol	Joback Method
hvap	53.74	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	2.608		Crippen Method
mcvol	117.930	ml/mol	McGowan Method
pc	4119.70	kPa	Joback Method
rinpol	1374.00		NIST Webbook
tb	532.15	K	Joback Method
tc	764.53	K	Joback Method
tf	360.50	K	Joback Method
vc	0.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.12	J/mol×K	532.15	Joback Method
cpg	294.10	J/mol×K	725.80	Joback Method
cpg	286.17	J/mol×K	687.07	Joback Method
cpg	277.69	J/mol×K	648.34	Joback Method
cpg	268.57	J/mol×K	609.61	Joback Method
cpg	258.75	J/mol×K	570.88	Joback Method
cpg	301.55	J/mol×K	764.53	Joback Method

dvisc	0.0000708	Pa×s	532.15	Joback Method
dvisc	0.0001055	Pa×s	503.54	Joback Method
dvisc	0.0001648	Pa×s	474.93	Joback Method
dvisc	0.0002727	Pa×s	446.32	Joback Method
dvisc	0.0004833	Pa×s	417.72	Joback Method
dvisc	0.0009319	Pa×s	389.11	Joback Method
dvisc	0.0019941	Pa×s	360.50	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18980002&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