tetrachloroguaiacol

Other names: 2,3,4,5-tetrachloro-6-methoxyphenol
Inchi: InChI=1S/C7H4Cl4O2/c1-13-7-5(11)3(9)2(8)4(10)6(7)12/h12H,1H3
InchiKey: YZZVKLJKDFFSFL-UHFFFAOYSA-N
Formula: C7H4Cl4O2
SMILES: COc1c(O)c(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 261.92

Physical Properties

Property code	Value	Unit	Source
gf	-225.39	kJ/mol	Joback Method
hf	-369.65	kJ/mol	Joback Method
hfus	30.13	kJ/mol	Joback Method
hvap	69.06	kJ/mol	Joback Method
log10ws	-4.02		Aqueous Solubility Prediction Method
log10ws	-4.02		Estimated Solubility Method
logp	4.014		Crippen Method
mcvol	146.430	ml/mol	McGowan Method
pc	3740.80	kPa	Joback Method
tb	658.92	K	Joback Method
tc	906.45	K	Joback Method
tf	498.78	K	Joback Method
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.46	J/mol×K	658.92	Joback Method
cpg	285.84	J/mol×K	700.17	Joback Method
cpg	291.84	J/mol×K	741.43	Joback Method
cpg	297.50	J/mol×K	782.68	Joback Method
cpg	302.89	J/mol×K	823.94	Joback Method
cpg	308.03	J/mol×K	865.19	Joback Method

cpg	312.99	J/mol×K	906.45	Joback Method
dvisc	0.0001877	Pa×s	498.78	Joback Method
dvisc	0.0001234	Pa×s	525.47	Joback Method
dvisc	0.0000845	Pa×s	552.16	Joback Method
dvisc	0.0000599	Pa×s	578.85	Joback Method
dvisc	0.0000438	Pa×s	605.54	Joback Method
dvisc	0.0000329	Pa×s	632.23	Joback Method
dvisc	0.0000252	Pa×s	658.92	Joback Method

Sources

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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