Phenol, 2,3,6-trichloro-

Other names: 2,3,6-Trichlorophenol
Inchi: InChI=1S/C6H3Cl3O/c7-3-1-2-4(8)6(10)5(3)9/h1-2,10H
InchiKey: XGCHAIDDPMFRLJ-UHFFFAOYSA-N
Formula: C6H3Cl3O
SMILES: Oc1c(Cl)ccc(Cl)c1Cl
Mol. weight [g/mol]: 197.45
CAS: 933-75-5

Physical Properties

Property code	Value	Unit	Source
gf	-97.62	kJ/mol	Joback Method
hf	-178.11	kJ/mol	Joback Method
hfus	22.93	kJ/mol	Joback Method
hvap	58.72	kJ/mol	Joback Method
log10ws	-2.64		Aqueous Solubility Prediction Method
log10ws	-2.64		Estimated Solubility Method
logp	3.352		Crippen Method
mcvol	114.230	ml/mol	McGowan Method
pc	4723.61	kPa	Joback Method
tb	566.23	K	Joback Method
tc	818.35	K	Joback Method
tf	410.32	K	Joback Method
vc	0.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.55	J/mol×K	566.23	Joback Method
cpg	209.69	J/mol×K	608.25	Joback Method
cpg	215.28	J/mol×K	650.27	Joback Method
cpg	220.38	J/mol×K	692.29	Joback Method
cpg	225.09	J/mol×K	734.31	Joback Method

cpg	229.51	J/mol×K	776.33	Joback Method
cpg	233.71	J/mol×K	818.35	Joback Method
dvisc	0.0008360	Pa×s	410.32	Joback Method
dvisc	0.0004792	Pa×s	436.31	Joback Method
dvisc	0.0002925	Pa×s	462.29	Joback Method
dvisc	0.0001881	Pa×s	488.28	Joback Method
dvisc	0.0001265	Pa×s	514.26	Joback Method
dvisc	0.0000884	Pa×s	540.25	Joback Method
dvisc	0.0000638	Pa×s	566.23	Joback Method

Sources

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
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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C933755&Units=SI

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