Phenol, 2,3,5,6-tetrachloro-

Other names: 2,3,5,6-Tetrachlorophenol
Inchi: InChI=1S/C6H2Cl4O/c7-2-1-3(8)5(10)6(11)4(2)9/h1,11H
InchiKey: KEWNKZNZRIAIAK-UHFFFAOYSA-N
Formula: C6H2Cl4O
SMILES: Oc1c(Cl)c(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]: 231.89
CAS: 935-95-5

Physical Properties

Property code	Value	Unit	Source
gf	-119.18	kJ/mol	Joback Method
hf	-205.32	kJ/mol	Joback Method
hfus	26.74	kJ/mol	Joback Method
hvap	63.77	kJ/mol	Joback Method
log10ws	-3.37		Aqueous Solubility Prediction Method
log10ws	-3.37		Estimated Solubility Method
logp	4.006		Crippen Method
mcvol	126.470	ml/mol	McGowan Method
pc	4403.25	kPa	Joback Method
rinpol	1511.00		NIST Webbook
rinpol	1515.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1551.00		NIST Webbook
rinpol	1511.00		NIST Webbook
rinpol	1545.00		NIST Webbook
rinpol	1536.00		NIST Webbook
rinpol	1530.00		NIST Webbook
ripol	2603.00		NIST Webbook
ripol	2553.00		NIST Webbook
ripol	2573.00		NIST Webbook
ripol	2615.00		NIST Webbook
ripol	2620.00		NIST Webbook
ripol	2598.00		NIST Webbook
ripol	2620.00		NIST Webbook
ripol	2553.00		NIST Webbook
tb	608.64	K	Joback Method

tc	865.32	K	Joback Method
tf	452.76	K	Joback Method
vc	0.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.56	J/mol×K	608.64	Joback Method
cpg	223.68	J/mol×K	651.42	Joback Method
cpg	228.36	J/mol×K	694.20	Joback Method
cpg	232.70	J/mol×K	736.98	Joback Method
cpg	236.77	J/mol×K	779.76	Joback Method
cpg	240.66	J/mol×K	822.54	Joback Method
cpg	244.46	J/mol×K	865.32	Joback Method
dvisc	0.0004365	Pa×s	452.76	Joback Method
dvisc	0.0002718	Pa×s	478.74	Joback Method
dvisc	0.0001777	Pa×s	504.72	Joback Method
dvisc	0.0001211	Pa×s	530.70	Joback Method
dvisc	0.0000855	Pa×s	556.68	Joback Method
dvisc	0.0000623	Pa×s	582.66	Joback Method
dvisc	0.0000467	Pa×s	608.64	Joback Method

Sources

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=C935955&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume