3,4,5,6-tetrachlorobenzene-1,2-diol

Inchi: InChI=1S/C6H2Cl4O2/c7-1-2(8)4(10)6(12)5(11)3(1)9/h11-12H
InchiKey: RRBMVWQICIXSEO-UHFFFAOYSA-N
Formula: C6H2Cl4O2
SMILES: Oc1c(O)c(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 247.89

Physical Properties

Property code	Value	Unit	Source
gf	-273.80	kJ/mol	Joback Method
hf	-382.63	kJ/mol	Joback Method
hfus	32.52	kJ/mol	Joback Method
hvap	76.78	kJ/mol	Joback Method
log10ws	-3.55		Aqueous Solubility Prediction Method
logp	3.711		Crippen Method
mcvol	132.340	ml/mol	McGowan Method
pc	5422.51	kPa	Joback Method
tb	689.26	K	Joback Method
tc	953.67	K	Joback Method
tf	564.48	K	Joback Method
vc	0.392	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.27	J/mol×K	689.26	Joback Method
cpg	251.42	J/mol×K	733.33	Joback Method
cpg	255.42	J/mol×K	777.40	Joback Method
cpg	259.44	J/mol×K	821.47	Joback Method
cpg	263.62	J/mol×K	865.54	Joback Method
cpg	268.15	J/mol×K	909.61	Joback Method
cpg	273.16	J/mol×K	953.67	Joback Method
dvisc	0.0000238	Pa×s	564.48	Joback Method
dvisc	0.0000158	Pa×s	585.28	Joback Method

dvisc	0.0000108	Pa×s	606.07	Joback Method
dvisc	0.0000076	Pa×s	626.87	Joback Method
dvisc	0.0000055	Pa×s	647.67	Joback Method
dvisc	0.0000040	Pa×s	668.46	Joback Method
dvisc	0.0000030	Pa×s	689.26	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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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