Phenol, 2,3,4,5-tetrachloro-, acetate

Other names: Acetic acid, 2,3,4,5-tetrachlorophenyl ester
Inchi: InChI=1S/C8H4Cl4O2/c1-3(13)14-5-2-4(9)6(10)8(12)7(5)11/h2H,1H3
InchiKey: QHRJCQOAJGBWRV-UHFFFAOYSA-N
Formula: C8H4Cl4O2
SMILES: CC(=O)Oc1cc(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 273.93
CAS: 4901-57-9

Physical Properties

Property code	Value	Unit	Source
gf	-191.27	kJ/mol	Joback Method
hf	-325.56	kJ/mol	Joback Method
hfus	28.54	kJ/mol	Joback Method
hvap	65.02	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	4.226		Crippen Method
mcvol	156.220	ml/mol	McGowan Method
pc	3028.94	kPa	Joback Method
rinpol	1694.00		NIST Webbook
rinpol	1679.00		NIST Webbook
rinpol	1679.00		NIST Webbook
ripol	2233.00		NIST Webbook
ripol	2233.00		NIST Webbook
tb	655.05	K	Joback Method
tc	895.37	K	Joback Method
tf	448.26	K	Joback Method
vc	0.596	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	294.91	J/mol×K	655.05	Joback Method
cpg	302.43	J/mol×K	695.10	Joback Method
cpg	309.43	J/mol×K	735.16	Joback Method

cpg	315.89	J/mol×K	775.21	Joback Method
cpg	321.82	J/mol×K	815.26	Joback Method
cpg	327.20	J/mol×K	855.31	Joback Method
cpg	332.02	J/mol×K	895.37	Joback Method
dvisc	0.0008237	Pa×s	448.26	Joback Method
dvisc	0.0006042	Pa×s	482.72	Joback Method
dvisc	0.0004619	Pa×s	517.19	Joback Method
dvisc	0.0003652	Pa×s	551.65	Joback Method
dvisc	0.0002968	Pa×s	586.12	Joback Method
dvisc	0.0002468	Pa×s	620.59	Joback Method
dvisc	0.0002093	Pa×s	655.05	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4901579&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume