Pentachlorophenyl acetate

Other names:	Phenol, pentachloro-, acetate
	Rabcon
	CPA
	Pentachlorophenol, O-acetyl-
	2,3,4,5,6-Pentachlorophenyl acetate
Inchi:	InChI=1S/C8H3Cl5O2/c1-2(14)15-8-6(12)4(10)3(9)5(11)7(8)13/h1H3
InchiKey:	RRYATXLRCBOQTJ-UHFFFAOYSA-N
Formula:	C8H3Cl5O2
SMILES:	CC(=O)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	308.37
CAS:	1441-02-7

Physical Properties

Property code	Value	Unit	Source
gf	-212.83	kJ/mol	Joback Method
hf	-352.77	kJ/mol	Joback Method
hfus	32.34	kJ/mol	Joback Method
hvap	70.07	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	4.879		Crippen Method
mcvol	168.460	ml/mol	McGowan Method
pc	2862.74	kPa	Joback Method
rinpol	1808.00		NIST Webbook
rinpol	1844.00		NIST Webbook
rinpol	1808.00		NIST Webbook
rinpol	1809.00		NIST Webbook
rinpol	1844.00		NIST Webbook
rinpol	1800.00		NIST Webbook
ripol	2401.00		NIST Webbook
tb	697.46	K	Joback Method
tc	941.22	K	Joback Method
tf	490.70	K	Joback Method
vc	0.644	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.58	J/mol×K	697.46	Joback Method
cpg	338.55	J/mol×K	900.59	Joback Method
cpg	334.04	J/mol×K	859.97	Joback Method
cpg	328.97	J/mol×K	819.34	Joback Method
cpg	323.36	J/mol×K	778.71	Joback Method
cpg	317.23	J/mol×K	738.09	Joback Method
cpg	342.51	J/mol×K	941.22	Joback Method
dvisc	0.0001913	Pa×s	697.46	Joback Method
dvisc	0.0002231	Pa×s	663.00	Joback Method
dvisc	0.0002646	Pa×s	628.54	Joback Method
dvisc	0.0003202	Pa×s	594.08	Joback Method
dvisc	0.0003967	Pa×s	559.62	Joback Method
dvisc	0.0005054	Pa×s	525.16	Joback Method
dvisc	0.0006662	Pa×s	490.70	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1441027&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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