PENTACHLOROPHENYL ACETATE

Other names:	2,3,4,5,6-Pentachlorophenyl acetate
	CPA
	Pentachlorophenol, O-acetyl-
	Phenol, pentachloro-, acetate
	Rabcon
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]:	308.38

Physical Properties

Property code	Value	Unit	Source
hfus	32.34	kJ/mol	Joback Method
ie	8.82	eV	Cheméo Relay (1.0)
log10ws	-5.81		Cheméo Relay (1.0)
logp	4.879		Crippen Method
mcvol	168.460	ml/mol	McGowan Method
rinpol	1809.00		NIST Webbook
rinpol	1808.00		NIST Webbook
rinpol	1844.00		NIST Webbook
rinpol	1808.00		NIST Webbook
rinpol	1800.00		NIST Webbook
rinpol	1844.00		NIST Webbook
rinpol	1800.00		NIST Webbook
ripol	2401.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.58	J/mol×K	697.46	Joback Method
cpg	342.51	J/mol×K	941.22	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
dvisc	0.0003202	Pa×s	594.08	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	0.0006662	Pa×s	490.70	Joback Method
dvisc	0.0003967	Pa×s	559.62	Joback Method
dvisc	0.0005054	Pa×s	525.16	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1441027&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hfus: Enthalpy of fusion at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
ripol: Polar retention indices