Chloroacetic acid, pentafluorophenyl ester

Inchi: InChI=1S/C8H2ClF5O2/c9-1-2(15)16-8-6(13)4(11)3(10)5(12)7(8)14/h1H2
InchiKey: VVKNQIGLUQLDPD-UHFFFAOYSA-N
Formula: C8H2ClF5O2
SMILES: O=C(CCl)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 260.55

Physical Properties

Property code	Value	Unit	Source
gf	-1139.16	kJ/mol	Joback Method
hf	-1270.36	kJ/mol	Joback Method
hfus	30.96	kJ/mol	Joback Method
hvap	48.44	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	2.526		Crippen Method
mcvol	128.350	ml/mol	McGowan Method
pc	2640.67	kPa	Joback Method
rinpol	1151.00		NIST Webbook
tb	544.09	K	Joback Method
tc	724.72	K	Joback Method
tf	373.97	K	Joback Method
vc	0.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.92	J/mol×K	544.09	Joback Method
cpg	282.94	J/mol×K	574.20	Joback Method
cpg	289.68	J/mol×K	604.30	Joback Method
cpg	296.14	J/mol×K	634.41	Joback Method
cpg	302.32	J/mol×K	664.51	Joback Method
cpg	308.19	J/mol×K	694.62	Joback Method
cpg	313.76	J/mol×K	724.72	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354605&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume