2-Chlorobenzoic acid, pentafluorophenyl ester

Inchi: InChI=1S/C13H4ClF5O2/c14-6-4-2-1-3-5(6)13(20)21-12-10(18)8(16)7(15)9(17)11(12)19/
InchiKey: OFSWADGNCDTNRE-UHFFFAOYSA-N
Formula: C13H4ClF5O2
SMILES: O=C(Oc1c(F)c(F)c(F)c(F)c1F)c1ccccc1Cl
Mol. weight [g/mol]: 322.62

Physical Properties

Property code	Value	Unit	Source
gf	-994.28	kJ/mol	Joback Method
hf	-1148.50	kJ/mol	Joback Method
hfus	37.56	kJ/mol	Joback Method
hvap	62.51	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	4.255		Crippen Method
mcvol	175.040	ml/mol	McGowan Method
pc	2246.13	kPa	Joback Method
rinpol	1674.00		NIST Webbook
rinpol	1674.00		NIST Webbook
tb	690.15	K	Joback Method
tc	895.37	K	Joback Method
tf	469.26	K	Joback Method
vc	0.711	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.76	J/mol×K	690.15	Joback Method
cpg	432.30	J/mol×K	724.35	Joback Method
cpg	441.18	J/mol×K	758.56	Joback Method
cpg	449.42	J/mol×K	792.76	Joback Method
cpg	457.02	J/mol×K	826.97	Joback Method
cpg	463.99	J/mol×K	861.17	Joback Method
cpg	470.33	J/mol×K	895.37	Joback Method

Sources

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=U360521&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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