4-Fluorobenzoic acid, 2-chlorophenyl ester

Inchi: InChI=1S/C13H8ClFO2/c14-11-3-1-2-4-12(11)17-13(16)9-5-7-10(15)8-6-9/h1-8H
InchiKey: ACJMGBBVOYNLCG-UHFFFAOYSA-N
Formula: C13H8ClFO2
SMILES: O=C(Oc1ccccc1Cl)c1ccc(F)cc1
Mol. weight [g/mol]: 250.65

Physical Properties

Property code	Value	Unit	Source
gf	-176.52	kJ/mol	Joback Method
hf	-318.18	kJ/mol	Joback Method
hfus	26.79	kJ/mol	Joback Method
hvap	63.13	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	3.698		Crippen Method
mcvol	167.960	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
rinpol	1735.00		NIST Webbook
tb	673.15	K	Joback Method
tc	913.93	K	Joback Method
tf	416.82	K	Joback Method
vc	0.638	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.42	J/mol×K	673.15	Joback Method
cpg	408.77	J/mol×K	713.28	Joback Method
cpg	420.11	J/mol×K	753.41	Joback Method
cpg	430.47	J/mol×K	793.54	Joback Method
cpg	439.89	J/mol×K	833.67	Joback Method
cpg	448.41	J/mol×K	873.80	Joback Method
cpg	456.07	J/mol×K	913.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299050&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
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