3-Fluorobenzoic acid, 2,3,4,6-tetrachlorophenyl ester

Inchi: InChI=1S/C13H5Cl4FO2/c14-8-5-9(15)12(11(17)10(8)16)20-13(19)6-2-1-3-7(18)4-6/h1-5

InchiKey: LPZMSZKUTBOUPJ-UHFFFAOYSA-N

Formula: C13H5Cl4FO2

SMILES: O=C(Oc1c(Cl)cc(Cl)c(Cl)c1Cl)c1cccc(F)c1

Mol. weight [g/mol]: 353.99

Physical Properties

Property code	Value	Unit	Source
gf	-241.20	kJ/mol	Joback Method
hf	-399.81	kJ/mol	Joback Method
hfus	38.22	kJ/mol	Joback Method
hvap	78.27	kJ/mol	Joback Method
log10ws	-6.63		Crippen Method
logp	5.659		Crippen Method
mcvol	204.680	ml/mol	McGowan Method
pc	2436.25	kPa	Joback Method
rinpol	2294.00		NIST Webbook
rinpol	2294.00		NIST Webbook
tb	800.38	K	Joback Method
tc	1049.98	K	Joback Method
tf	544.14	K	Joback Method
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	452.35	J/mol×K	800.38	Joback Method
cpg	460.90	J/mol×K	841.98	Joback Method
cpg	468.57	J/mol×K	883.58	Joback Method
cpg	475.35	J/mol×K	925.18	Joback Method
cpg	481.29	J/mol×K	966.78	Joback Method
cpg	486.39	J/mol×K	1008.38	Joback Method
cpg	490.68	J/mol×K	1049.98	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=U355668&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