3-Chloro-2-fluorobenzoic acid, 2,4-dichloro-6-formylphenyl ester

Inchi: InChI=1S/C14H6Cl3FO3/c15-8-4-7(6-19)13(11(17)5-8)21-14(20)9-2-1-3-10(16)12(9)18/h

InchiKey: SNCOJQXUIMUEQY-UHFFFAOYSA-N

Formula: C14H6Cl3FO3

SMILES: O=Cc1cc(Cl)cc(Cl)c1OC(=O)c1cccc(Cl)c1F

Mol. weight [g/mol]: 347.55

Physical Properties

Property code	Value	Unit	Source
gf	-320.37	kJ/mol	Joback Method
hf	-490.29	kJ/mol	Joback Method
hfus	38.90	kJ/mol	Joback Method
hvap	82.83	kJ/mol	Joback Method
log10ws	-6.19		Crippen Method
logp	4.818		Crippen Method
mcvol	208.100	ml/mol	McGowan Method
pc	2472.73	kPa	Joback Method
rinpol	2432.00		NIST Webbook
tb	834.49	K	Joback Method
tc	1077.69	K	Joback Method
tf	567.49	K	Joback Method
vc	0.809	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.02	J/mol×K	834.49	Joback Method
cpg	499.39	J/mol×K	875.02	Joback Method
cpg	506.85	J/mol×K	915.56	Joback Method
cpg	513.41	J/mol×K	956.09	Joback Method
cpg	519.10	J/mol×K	996.63	Joback Method
cpg	523.93	J/mol×K	1037.16	Joback Method
cpg	527.92	J/mol×K	1077.69	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=U357338&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