3-Chloro-2-fluorobenzoic acid, 3,4-dichlorophenyl ester

Inchi: InChI=1S/C13H6Cl3FO2/c14-9-5-4-7(6-11(9)16)19-13(18)8-2-1-3-10(15)12(8)17/h1-6H

InchiKey: UQUHAAHZWIDVOX-UHFFFAOYSA-N

Formula: C13H6Cl3FO2

SMILES: O=C(Oc1ccc(Cl)c(Cl)c1)c1cccc(Cl)c1F

Mol. weight [g/mol]: 319.54

Physical Properties

Property code	Value	Unit	Source
gf	-219.64	kJ/mol	Joback Method
hf	-372.60	kJ/mol	Joback Method
hfus	34.41	kJ/mol	Joback Method
hvap	73.23	kJ/mol	Joback Method
log10ws	-5.95		Crippen Method
logp	5.005		Crippen Method
mcvol	192.440	ml/mol	McGowan Method
pc	2566.29	kPa	Joback Method
rinpol	2292.00		NIST Webbook
rinpol	2292.00		NIST Webbook
tb	757.97	K	Joback Method
tc	1004.92	K	Joback Method
tf	501.70	K	Joback Method
vc	0.737	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.57	J/mol×K	757.97	Joback Method
cpg	445.33	J/mol×K	799.13	Joback Method
cpg	454.17	J/mol×K	840.29	Joback Method
cpg	462.11	J/mol×K	881.45	Joback Method
cpg	469.18	J/mol×K	922.61	Joback Method
cpg	475.40	J/mol×K	963.76	Joback Method
cpg	480.80	J/mol×K	1004.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357733&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

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