3-Chloro-2-fluorobenzoic acid, 3,5-difluophenyl ester

Inchi: InChI=1S/C13H6ClF3O2/c14-11-3-1-2-10(12(11)17)13(18)19-9-5-7(15)4-8(16)6-9/h1-6H

InchiKey: AFHBXBRIHLALFI-UHFFFAOYSA-N

Formula: C13H6ClF3O2

SMILES: O=C(Oc1cc(F)cc(F)c1)c1cccc(Cl)c1F

Mol. weight [g/mol]: 286.63

Physical Properties

Property code	Value	Unit	Source
gf	-585.40	kJ/mol	Joback Method
hf	-733.34	kJ/mol	Joback Method
hfus	32.18	kJ/mol	Joback Method
hvap	62.82	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	3.976		Crippen Method
mcvol	171.500	ml/mol	McGowan Method
pc	2525.19	kPa	Joback Method
rinpol	1796.00		NIST Webbook
rinpol	1796.00		NIST Webbook
tb	681.65	K	Joback Method
tc	903.02	K	Joback Method
tf	443.04	K	Joback Method
vc	0.674	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.71	J/mol×K	681.65	Joback Method
cpg	420.52	J/mol×K	718.55	Joback Method
cpg	430.53	J/mol×K	755.44	Joback Method
cpg	439.75	J/mol×K	792.34	Joback Method
cpg	448.20	J/mol×K	829.23	Joback Method
cpg	455.90	J/mol×K	866.13	Joback Method
cpg	462.87	J/mol×K	903.02	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=U357722&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