3-Chloro-2-fluorobenzoic acid, 3-methylphenyl ester

Inchi: InChI=1S/C14H10ClFO2/c1-9-4-2-5-10(8-9)18-14(17)11-6-3-7-12(15)13(11)16/h2-8H,1H

InchiKey: VRSWPYUREXWJDA-UHFFFAOYSA-N

Formula: C14H10ClFO2

SMILES: Cc1cccc(OC(=O)c2cccc(Cl)c2F)c1

Mol. weight [g/mol]: 264.68

Physical Properties

Property code	Value	Unit	Source
gf	-177.73	kJ/mol	Joback Method
hf	-350.29	kJ/mol	Joback Method
hfus	29.00	kJ/mol	Joback Method
hvap	66.02	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	4.007		Crippen Method
mcvol	182.050	ml/mol	McGowan Method
pc	2548.19	kPa	Joback Method
rinpol	2004.00		NIST Webbook
tb	701.01	K	Joback Method
tc	937.70	K	Joback Method
tf	440.61	K	Joback Method
vc	0.695	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.13	J/mol×K	701.01	Joback Method
cpg	457.90	J/mol×K	740.46	Joback Method
cpg	469.67	J/mol×K	779.91	Joback Method
cpg	480.47	J/mol×K	819.35	Joback Method
cpg	490.32	J/mol×K	858.80	Joback Method
cpg	499.25	J/mol×K	898.25	Joback Method
cpg	507.30	J/mol×K	937.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357727&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