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

Inchi: InChI=1S/C14H10ClFO3/c1-18-9-5-7-10(8-6-9)19-14(17)11-3-2-4-12(15)13(11)16/h2-8H

InchiKey: LBGISFBWNOLNTA-UHFFFAOYSA-N

Formula: C14H10ClFO3

SMILES: COc1ccc(OC(=O)c2cccc(Cl)c2F)cc1

Mol. weight [g/mol]: 280.68

Physical Properties

Property code	Value	Unit	Source
gf	-282.73	kJ/mol	Joback Method
hf	-482.51	kJ/mol	Joback Method
hfus	30.18	kJ/mol	Joback Method
hvap	68.43	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	3.707		Crippen Method
mcvol	187.920	ml/mol	McGowan Method
pc	2505.01	kPa	Joback Method
rinpol	2174.00		NIST Webbook
tb	723.43	K	Joback Method
tc	956.74	K	Joback Method
tf	462.84	K	Joback Method
vc	0.713	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.64	J/mol×K	723.43	Joback Method
cpg	482.10	J/mol×K	762.31	Joback Method
cpg	493.55	J/mol×K	801.20	Joback Method
cpg	504.01	J/mol×K	840.08	Joback Method
cpg	513.49	J/mol×K	878.97	Joback Method
cpg	521.99	J/mol×K	917.85	Joback Method
cpg	529.53	J/mol×K	956.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357730&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