3-Chloro-2-fluorobenzoic acid, 4-methoxy-2-methylbutyl ester

Inchi: InChI=1S/C13H16ClFO3/c1-9(6-7-17-2)8-18-13(16)10-4-3-5-11(14)12(10)15/h3-5,9H,6-8

InchiKey: SGMQPTHYGIDLIJ-UHFFFAOYSA-N

Formula: C13H16ClFO3

SMILES: COCCC(C)COC(=O)c1cccc(Cl)c1F

Mol. weight [g/mol]: 274.72

Physical Properties

Property code	Value	Unit	Source
gf	-396.37	kJ/mol	Joback Method
hf	-692.21	kJ/mol	Joback Method
hfus	30.42	kJ/mol	Joback Method
hvap	62.88	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.308		Crippen Method
mcvol	197.590	ml/mol	McGowan Method
pc	2047.46	kPa	Joback Method
rinpol	1868.00		NIST Webbook
tb	668.45	K	Joback Method
tc	870.17	K	Joback Method
tf	397.63	K	Joback Method
vc	0.758	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	505.07	J/mol×K	668.45	Joback Method
cpg	518.90	J/mol×K	702.07	Joback Method
cpg	531.93	J/mol×K	735.69	Joback Method
cpg	544.18	J/mol×K	769.31	Joback Method
cpg	555.64	J/mol×K	802.93	Joback Method
cpg	566.33	J/mol×K	836.55	Joback Method
cpg	576.24	J/mol×K	870.17	Joback Method

Sources

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=U360584&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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