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

Inchi: InChI=1S/C16H14ClFO2/c1-10(2)11-6-8-12(9-7-11)20-16(19)13-4-3-5-14(17)15(13)18/h3
InchiKey: KKWCTQWJMJGYFU-UHFFFAOYSA-N
Formula: C16H14ClFO2
SMILES: CC(C)c1ccc(OC(=O)c2cccc(Cl)c2F)cc1
Mol. weight [g/mol]: 292.73

Physical Properties

Property code	Value	Unit	Source
gf	-163.33	kJ/mol	Joback Method
hf	-396.85	kJ/mol	Joback Method
hfus	30.65	kJ/mol	Joback Method
hvap	70.08	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	4.822		Crippen Method
mcvol	210.230	ml/mol	McGowan Method
pc	2133.46	kPa	Joback Method
rinpol	2184.00		NIST Webbook
rinpol	2184.00		NIST Webbook
tb	746.33	K	Joback Method
tc	978.53	K	Joback Method
tf	448.15	K	Joback Method
vc	0.800	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	549.74	J/mol×K	746.33	Joback Method
cpg	563.68	J/mol×K	785.03	Joback Method
cpg	576.52	J/mol×K	823.73	Joback Method
cpg	588.28	J/mol×K	862.43	Joback Method
cpg	599.02	J/mol×K	901.13	Joback Method
cpg	608.76	J/mol×K	939.83	Joback Method
cpg	617.54	J/mol×K	978.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357333&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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