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

Inchi: InChI=1S/C16H14ClFO2/c1-2-6-11-7-3-4-10-14(11)20-16(19)12-8-5-9-13(17)15(12)18/h3

InchiKey: ZFJBUZDFPACSNX-UHFFFAOYSA-N

Formula: C16H14ClFO2

SMILES: CCCc1ccccc1OC(=O)c1cccc(Cl)c1F

Mol. weight [g/mol]: 292.73

Physical Properties

Property code	Value	Unit	Source
gf	-160.89	kJ/mol	Joback Method
hf	-391.57	kJ/mol	Joback Method
hfus	34.17	kJ/mol	Joback Method
hvap	70.47	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	4.651		Crippen Method
mcvol	210.230	ml/mol	McGowan Method
pc	2117.78	kPa	Joback Method
rinpol	2093.00		NIST Webbook
rinpol	2093.00		NIST Webbook
tb	746.77	K	Joback Method
tc	974.84	K	Joback Method
tf	463.15	K	Joback Method
vc	0.806	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	549.16	J/mol×K	746.77	Joback Method
cpg	562.84	J/mol×K	784.78	Joback Method
cpg	575.47	J/mol×K	822.79	Joback Method
cpg	587.09	J/mol×K	860.80	Joback Method
cpg	597.71	J/mol×K	898.81	Joback Method
cpg	607.39	J/mol×K	936.83	Joback Method
cpg	616.16	J/mol×K	974.84	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=U360585&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