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

Inchi: InChI=1S/C12H14ClFO2/c1-3-5-8(2)16-12(15)9-6-4-7-10(13)11(9)14/h4,6-8H,3,5H2,1-2H
InchiKey: RWVDQAVTFWQLPA-UHFFFAOYSA-N
Formula: C12H14ClFO2
SMILES: CCCC(C)OC(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 244.69

Physical Properties

Property code	Value	Unit	Source
gf	-299.79	kJ/mol	Joback Method
hf	-539.35	kJ/mol	Joback Method
hfus	26.64	kJ/mol	Joback Method
hvap	58.24	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	3.825		Crippen Method
mcvol	177.630	ml/mol	McGowan Method
pc	2274.07	kPa	Joback Method
rinpol	1587.00		NIST Webbook
rinpol	1587.00		NIST Webbook
tb	623.15	K	Joback Method
tc	829.57	K	Joback Method
tf	364.13	K	Joback Method
vc	0.684	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.19	J/mol×K	623.15	Joback Method
cpg	442.65	J/mol×K	657.55	Joback Method
cpg	455.34	J/mol×K	691.96	Joback Method
cpg	467.28	J/mol×K	726.36	Joback Method
cpg	478.49	J/mol×K	760.77	Joback Method
cpg	488.97	J/mol×K	795.17	Joback Method
cpg	498.75	J/mol×K	829.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357721&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