3-Chloro-2-fluorobenzoic acid, pentyl ester

Inchi: InChI=1S/C12H14ClFO2/c1-2-3-4-8-16-12(15)9-6-5-7-10(13)11(9)14/h5-7H,2-4,8H2,1H3
InchiKey: JNSCMNATFSNCPL-UHFFFAOYSA-N
Formula: C12H14ClFO2
SMILES: CCCCCOC(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 244.69

Physical Properties

Property code	Value	Unit	Source
gf	-297.35	kJ/mol	Joback Method
hf	-534.07	kJ/mol	Joback Method
hfus	30.16	kJ/mol	Joback Method
hvap	58.63	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	3.826		Crippen Method
mcvol	177.630	ml/mol	McGowan Method
pc	2256.81	kPa	Joback Method
rinpol	1688.00		NIST Webbook
rinpol	1688.00		NIST Webbook
tb	623.59	K	Joback Method
tc	826.11	K	Joback Method
tf	379.13	K	Joback Method
vc	0.691	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.72	J/mol×K	623.59	Joback Method
cpg	441.88	J/mol×K	657.34	Joback Method
cpg	454.31	J/mol×K	691.10	Joback Method
cpg	466.03	J/mol×K	724.85	Joback Method
cpg	477.05	J/mol×K	758.60	Joback Method
cpg	487.39	J/mol×K	792.35	Joback Method
cpg	497.05	J/mol×K	826.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338881&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