D-Alanine, N-(3-chloro-2-fluorobenzoyl)-, hexyl ester

Inchi: InChI=1S/C16H21ClFNO3/c1-3-4-5-6-10-22-16(21)11(2)19-15(20)12-8-7-9-13(17)14(12)18/h7-9,11H,3-6,10H2,1-2H3,(H,19,20)/t11-/m1/s1

InchiKey: LJOKYNXLEWIOSS-UHFFFAOYSA-N

Formula: C16H21ClFNO3

SMILES: CCCCCCOC(=O)C(C)NC(=O)c1cccc(Cl)c1F

Mol. weight [g/mol]: 329.79

Physical Properties

Property code	Value	Unit	Source
gf	-305.64	kJ/mol	Joback Method
hf	-681.02	kJ/mol	Joback Method
hfus	43.70	kJ/mol	Joback Method
hvap	80.33	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	3.721		Crippen Method
mcvol	245.540	ml/mol	McGowan Method
pc	1728.90	kPa	Joback Method
rinpol	2319.00		NIST Webbook
tb	818.71	K	Joback Method
tc	1024.18	K	Joback Method
tf	511.80	K	Joback Method
vc	0.950	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.85	J/mol×K	818.71	Joback Method
cpg	723.12	J/mol×K	852.95	Joback Method
cpg	735.43	J/mol×K	887.20	Joback Method
cpg	746.80	J/mol×K	921.44	Joback Method
cpg	757.26	J/mol×K	955.69	Joback Method
cpg	766.84	J/mol×K	989.93	Joback Method
cpg	775.55	J/mol×K	1024.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348339&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