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

Inchi: InChI=1S/C16H21ClFNO3/c1-10(2)6-5-9-22-16(21)11(3)19-15(20)12-7-4-8-13(17)14(12)
InchiKey: ZJKYSVPGRXJVMS-UHFFFAOYSA-N
Formula: C16H21ClFNO3
SMILES: CC(C)CCCOC(=O)C(C)NC(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 329.79

Physical Properties

Property code	Value	Unit	Source
gf	-308.08	kJ/mol	Joback Method
hf	-686.30	kJ/mol	Joback Method
hfus	40.17	kJ/mol	Joback Method
hvap	79.94	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	3.577		Crippen Method
mcvol	245.540	ml/mol	McGowan Method
pc	1740.46	kPa	Joback Method
rinpol	2270.00		NIST Webbook
tb	818.27	K	Joback Method
tc	1026.17	K	Joback Method
tf	496.80	K	Joback Method
vc	0.944	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.42	J/mol×K	818.27	Joback Method
cpg	723.84	J/mol×K	852.92	Joback Method
cpg	736.26	J/mol×K	887.57	Joback Method
cpg	747.72	J/mol×K	922.22	Joback Method
cpg	758.22	J/mol×K	956.87	Joback Method
cpg	767.81	J/mol×K	991.52	Joback Method
cpg	776.51	J/mol×K	1026.17	Joback Method

Sources

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=U348338&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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