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

Inchi: InChI=1S/C28H45ClFNO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22-34-28(33)23

InchiKey: GAIRTYDLSHPJBM-UHFFFAOYSA-N

Formula: C28H45ClFNO3

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

Mol. weight [g/mol]: 498.11

Physical Properties

Property code	Value	Unit	Source
gf	-204.60	kJ/mol	Joback Method
hf	-928.70	kJ/mol	Joback Method
hfus	74.78	kJ/mol	Joback Method
hvap	107.04	kJ/mol	Joback Method
log10ws	-10.18		Crippen Method
logp	8.402		Crippen Method
mcvol	414.620	ml/mol	McGowan Method
pc	790.37	kPa	Joback Method
rinpol	3566.00		NIST Webbook
tb	1093.27	K	Joback Method
tc	1353.36	K	Joback Method
tf	647.04	K	Joback Method
vc	1.621	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1432.37	J/mol×K	1093.27	Joback Method
cpg	1449.58	J/mol×K	1136.62	Joback Method
cpg	1464.96	J/mol×K	1179.97	Joback Method
cpg	1478.64	J/mol×K	1223.31	Joback Method
cpg	1490.73	J/mol×K	1266.66	Joback Method
cpg	1501.36	J/mol×K	1310.01	Joback Method
cpg	1510.65	J/mol×K	1353.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348342&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