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

Inchi: InChI=1S/C27H43ClFNO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21-33-27(32)22(2)30-26(31)23-18-19-25(29)24(28)20-23/h18-20,22H,3-17,21H2,1-2H3,(H,30,31)/t22-/m1/s1

InchiKey: SJGGQYJKHJDRDW-UHFFFAOYSA-N

Formula: C27H43ClFNO3

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

Mol. weight [g/mol]: 484.09

Physical Properties

Property code	Value	Unit	Source
gf	-213.02	kJ/mol	Joback Method
hf	-908.06	kJ/mol	Joback Method
hfus	72.19	kJ/mol	Joback Method
hvap	104.81	kJ/mol	Joback Method
log10ws	-9.76		Crippen Method
logp	8.012		Crippen Method
mcvol	400.530	ml/mol	McGowan Method
pc	834.83	kPa	Joback Method
rinpol	3348.00		NIST Webbook
tb	1070.39	K	Joback Method
tc	1319.77	K	Joback Method
tf	635.77	K	Joback Method
vc	1.565	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1369.47	J/mol×K	1070.39	Joback Method
cpg	1386.19	J/mol×K	1111.95	Joback Method
cpg	1401.23	J/mol×K	1153.52	Joback Method
cpg	1414.68	J/mol×K	1195.08	Joback Method
cpg	1426.63	J/mol×K	1236.64	Joback Method
cpg	1437.20	J/mol×K	1278.20	Joback Method
cpg	1446.49	J/mol×K	1319.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348341&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

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

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