L-Valine, N-(3-chloro-2-fluorobenzoyl)-, pentadecyl ester

Inchi: InChI=1S/C27H43ClFNO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-20-33-27(32)25(21(2)3)30-26(31)22-17-18-23(28)24(29)19-22/h17-19,21,25H,4-16,20H2,1-3H3,(H,30,31)/t25-/m0/s1

InchiKey: RZMXPUJOBAPPJQ-UHFFFAOYSA-N

Formula: C27H43ClFNO3

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

Mol. weight [g/mol]: 484.09

Physical Properties

Property code	Value	Unit	Source
gf	-215.46	kJ/mol	Joback Method
hf	-913.34	kJ/mol	Joback Method
hfus	68.66	kJ/mol	Joback Method
hvap	104.43	kJ/mol	Joback Method
log10ws	-9.52		Crippen Method
logp	7.868		Crippen Method
mcvol	400.530	ml/mol	McGowan Method
pc	838.70	kPa	Joback Method
rinpol	3350.00		NIST Webbook
rinpol	3350.00		NIST Webbook
tb	1069.95	K	Joback Method
tc	1317.51	K	Joback Method
tf	620.77	K	Joback Method
vc	1.560	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1369.66	J/mol×K	1069.95	Joback Method
cpg	1386.17	J/mol×K	1111.21	Joback Method
cpg	1401.00	J/mol×K	1152.47	Joback Method
cpg	1414.24	J/mol×K	1193.73	Joback Method
cpg	1425.99	J/mol×K	1234.99	Joback Method
cpg	1436.36	J/mol×K	1276.25	Joback Method
cpg	1445.44	J/mol×K	1317.51	Joback Method

Sources

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=U346547&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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