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

Inchi: InChI=1S/C29H47ClFNO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22-35-29(34)27(2

InchiKey: BGUNZGXMCCLXBJ-UHFFFAOYSA-N

Formula: C29H47ClFNO3

SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(N=C(O)c1cccc(Cl)c1F)C(C)C

Mol. weight [g/mol]: 512.14

Physical Properties

Property code	Value	Unit	Source
hf	-975.31	kJ/mol	Joback Method
hvap	115.77	kJ/mol	Joback Method
log10ws	-9.90		Crippen Method
logp	9.223		Crippen Method
mcvol	428.710	ml/mol	McGowan Method
pc	719.14	kPa	Joback Method
rinpol	3571.00		NIST Webbook
rinpol	3571.00		NIST Webbook
tb	1180.41	K	Joback Method
tc	1486.20	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346549&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

hf: Enthalpy of formation 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