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

Inchi: InChI=1S/C18H25ClFNO3/c1-11(2)7-6-10-24-18(23)16(12(3)4)21-17(22)13-8-5-9-14(19)

InchiKey: TYBJGMNJVKIAJU-UHFFFAOYSA-N

Formula: C18H25ClFNO3

SMILES: CC(C)CCCOC(=O)C(N=C(O)c1cccc(Cl)c1F)C(C)C

Mol. weight [g/mol]: 357.85

Physical Properties

Property code	Value	Unit	Source
hf	-753.55	kJ/mol	Joback Method
hvap	90.89	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	4.788		Crippen Method
mcvol	273.720	ml/mol	McGowan Method
pc	1408.01	kPa	Joback Method
rinpol	2369.00		NIST Webbook
rinpol	2369.00		NIST Webbook
tb	928.29	K	Joback Method
tc	1142.40	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346543&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

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