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

Inchi: InChI=1S/C28H45ClFNO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21-34-28(33)26(22(2

InchiKey: QQBWPQXGUITAQF-UHFFFAOYSA-N

Formula: C28H45ClFNO3

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

Mol. weight [g/mol]: 498.11

Physical Properties

Property code	Value	Unit	Source
gf	-207.04	kJ/mol	Joback Method
hf	-933.98	kJ/mol	Joback Method
hfus	71.26	kJ/mol	Joback Method
hvap	106.65	kJ/mol	Joback Method
log10ws	-9.94		Crippen Method
logp	8.258		Crippen Method
mcvol	414.620	ml/mol	McGowan Method
pc	793.94	kPa	Joback Method
rinpol	3451.00		NIST Webbook
rinpol	3451.00		NIST Webbook
tb	1092.83	K	Joback Method
tc	1350.59	K	Joback Method
tf	632.04	K	Joback Method
vc	1.615	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1432.50	J/mol×K	1092.83	Joback Method
cpg	1449.45	J/mol×K	1135.79	Joback Method
cpg	1464.58	J/mol×K	1178.75	Joback Method
cpg	1478.02	J/mol×K	1221.71	Joback Method
cpg	1489.88	J/mol×K	1264.67	Joback Method
cpg	1500.28	J/mol×K	1307.63	Joback Method
cpg	1509.34	J/mol×K	1350.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346548&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