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

Inchi: InChI=1S/C22H33ClFNO3/c1-4-5-6-7-8-9-10-11-15-28-22(27)20(16(2)3)25-21(26)17-13-

InchiKey: WZBKOACPSDODKV-UHFFFAOYSA-N

Formula: C22H33ClFNO3

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

Mol. weight [g/mol]: 413.95

Physical Properties

Property code	Value	Unit	Source
gf	-257.56	kJ/mol	Joback Method
hf	-810.14	kJ/mol	Joback Method
hfus	55.71	kJ/mol	Joback Method
hvap	93.30	kJ/mol	Joback Method
log10ws	-7.43		Crippen Method
logp	5.917		Crippen Method
mcvol	330.080	ml/mol	McGowan Method
pc	1131.38	kPa	Joback Method
rinpol	2816.00		NIST Webbook
tb	955.55	K	Joback Method
tc	1170.82	K	Joback Method
tf	564.42	K	Joback Method
vc	1.280	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1061.32	J/mol×K	955.55	Joback Method
cpg	1076.20	J/mol×K	991.43	Joback Method
cpg	1089.83	J/mol×K	1027.31	Joback Method
cpg	1102.27	J/mol×K	1063.19	Joback Method
cpg	1113.55	J/mol×K	1099.07	Joback Method
cpg	1123.72	J/mol×K	1134.94	Joback Method
cpg	1132.85	J/mol×K	1170.82	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=U346544&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