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

Inchi: InChI=1S/C23H35ClFNO3/c1-4-5-6-7-8-9-10-11-12-16-29-23(28)21(17(2)3)26-22(27)18-

InchiKey: IWDFXPNAANJEFZ-UHFFFAOYSA-N

Formula: C23H35ClFNO3

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

Mol. weight [g/mol]: 427.98

Physical Properties

Property code	Value	Unit	Source
gf	-249.14	kJ/mol	Joback Method
hf	-830.78	kJ/mol	Joback Method
hfus	58.30	kJ/mol	Joback Method
hvap	95.52	kJ/mol	Joback Method
log10ws	-7.84		Crippen Method
logp	6.308		Crippen Method
mcvol	344.170	ml/mol	McGowan Method
pc	1061.71	kPa	Joback Method
rinpol	2922.00		NIST Webbook
rinpol	2922.00		NIST Webbook
tb	978.43	K	Joback Method
tc	1197.94	K	Joback Method
tf	575.69	K	Joback Method
vc	1.335	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1122.07	J/mol×K	978.43	Joback Method
cpg	1137.22	J/mol×K	1015.02	Joback Method
cpg	1151.05	J/mol×K	1051.60	Joback Method
cpg	1163.63	J/mol×K	1088.19	Joback Method
cpg	1175.00	J/mol×K	1124.77	Joback Method
cpg	1185.23	J/mol×K	1161.36	Joback Method
cpg	1194.36	J/mol×K	1197.94	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346545&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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