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

Inchi: InChI=1S/C23H36FNO3/c1-4-5-6-7-8-9-10-11-12-16-28-23(27)21(18(2)3)25-22(26)19-14
InchiKey: CGSTUZILBBQLCE-UHFFFAOYSA-N
Formula: C23H36FNO3
SMILES: CCCCCCCCCCCOC(=O)C(NC(=O)c1cccc(F)c1)C(C)C
Mol. weight [g/mol]: 393.54

Physical Properties

Property code	Value	Unit	Source
gf	-227.58	kJ/mol	Joback Method
hf	-803.57	kJ/mol	Joback Method
hfus	54.50	kJ/mol	Joback Method
hvap	90.47	kJ/mol	Joback Method
log10ws	-7.16		Crippen Method
logp	5.654		Crippen Method
mcvol	331.930	ml/mol	McGowan Method
pc	1098.62	kPa	Joback Method
rinpol	2733.00		NIST Webbook
rinpol	2733.00		NIST Webbook
tb	936.02	K	Joback Method
tc	1146.73	K	Joback Method
tf	533.25	K	Joback Method
vc	1.286	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1097.10	J/mol×K	936.02	Joback Method
cpg	1113.45	J/mol×K	971.14	Joback Method
cpg	1128.53	J/mol×K	1006.26	Joback Method
cpg	1142.38	J/mol×K	1041.38	Joback Method
cpg	1155.07	J/mol×K	1076.50	Joback Method
cpg	1166.65	J/mol×K	1111.61	Joback Method
cpg	1177.16	J/mol×K	1146.73	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346678&Units=SI

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