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

Inchi: InChI=1S/C28H46FNO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21-33-28(32)26(23(2)3
InchiKey: COZXTPCIOBMDSV-UHFFFAOYSA-N
Formula: C28H46FNO3
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(NC(=O)c1cccc(F)c1)C(C)C
Mol. weight [g/mol]: 463.67

Physical Properties

Property code	Value	Unit	Source
gf	-185.48	kJ/mol	Joback Method
hf	-906.77	kJ/mol	Joback Method
hfus	67.45	kJ/mol	Joback Method
hvap	101.61	kJ/mol	Joback Method
log10ws	-9.25		Crippen Method
logp	7.605		Crippen Method
mcvol	402.380	ml/mol	McGowan Method
pc	817.73	kPa	Joback Method
rinpol	3252.00		NIST Webbook
rinpol	3252.00		NIST Webbook
tb	1050.42	K	Joback Method
tc	1293.97	K	Joback Method
tf	589.60	K	Joback Method
vc	1.567	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1409.01	J/mol×K	1050.42	Joback Method
cpg	1427.18	J/mol×K	1091.01	Joback Method
cpg	1443.64	J/mol×K	1131.60	Joback Method
cpg	1458.50	J/mol×K	1172.20	Joback Method
cpg	1471.85	J/mol×K	1212.79	Joback Method
cpg	1483.81	J/mol×K	1253.38	Joback Method
cpg	1494.48	J/mol×K	1293.97	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=U346682&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