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

Inchi: InChI=1S/C29H48FNO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22-34-29(33)27(24(
InchiKey: HWLOJHLJSPENDU-UHFFFAOYSA-N
Formula: C29H48FNO3
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(NC(=O)c1cccc(F)c1)C(C)C
Mol. weight [g/mol]: 477.69

Physical Properties

Property code	Value	Unit	Source
gf	-177.06	kJ/mol	Joback Method
hf	-927.41	kJ/mol	Joback Method
hfus	70.04	kJ/mol	Joback Method
hvap	103.83	kJ/mol	Joback Method
log10ws	-9.67		Crippen Method
logp	7.995		Crippen Method
mcvol	416.470	ml/mol	McGowan Method
pc	774.61	kPa	Joback Method
rinpol	3352.00		NIST Webbook
rinpol	3352.00		NIST Webbook
tb	1073.30	K	Joback Method
tc	1327.12	K	Joback Method
tf	600.87	K	Joback Method
vc	1.623	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1472.57	J/mol×K	1073.30	Joback Method
cpg	1491.24	J/mol×K	1115.60	Joback Method
cpg	1508.07	J/mol×K	1157.91	Joback Method
cpg	1523.19	J/mol×K	1200.21	Joback Method
cpg	1536.71	J/mol×K	1242.52	Joback Method
cpg	1548.77	J/mol×K	1284.82	Joback Method
cpg	1559.49	J/mol×K	1327.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346683&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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