L-Valine, N-(4-fluorobenzoyl)-, pentadecyl ester

Inchi: InChI=1S/C27H44FNO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-21-32-27(31)25(22(2)3)29

InchiKey: LEBDECNEEBYPME-UHFFFAOYSA-N

Formula: C27H44FNO3

SMILES: CCCCCCCCCCCCCCCOC(=O)C(NC(=O)c1ccc(F)cc1)C(C)C

Mol. weight [g/mol]: 449.64

Physical Properties

Property code	Value	Unit	Source
gf	-193.90	kJ/mol	Joback Method
hf	-886.13	kJ/mol	Joback Method
hfus	64.86	kJ/mol	Joback Method
hvap	99.38	kJ/mol	Joback Method
log10ws	-8.83		Crippen Method
logp	7.215		Crippen Method
mcvol	388.290	ml/mol	McGowan Method
pc	864.54	kPa	Joback Method
rinpol	3153.00		NIST Webbook
rinpol	3153.00		NIST Webbook
tb	1027.54	K	Joback Method
tc	1262.18	K	Joback Method
tf	578.33	K	Joback Method
vc	1.510	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1345.79	J/mol×K	1027.54	Joback Method
cpg	1363.51	J/mol×K	1066.65	Joback Method
cpg	1379.64	J/mol×K	1105.75	Joback Method
cpg	1394.26	J/mol×K	1144.86	Joback Method
cpg	1407.46	J/mol×K	1183.96	Joback Method
cpg	1419.33	J/mol×K	1223.07	Joback Method
cpg	1429.97	J/mol×K	1262.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346674&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

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