L-Valine, N-(3-trifluoromethylbenzoyl)-, tetradecyl ester

Inchi: InChI=1S/C27H42F3NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-19-34-26(33)24(21(2)3)31-2
InchiKey: HIPYJRUZLYMGBE-UHFFFAOYSA-N
Formula: C27H42F3NO3
SMILES: CCCCCCCCCCCCCCOC(=O)C(NC(=O)c1cccc(C(F)(F)F)c1)C(C)C
Mol. weight [g/mol]: 485.62

Physical Properties

Property code	Value	Unit	Source
gf	-580.68	kJ/mol	Joback Method
hf	-1287.10	kJ/mol	Joback Method
hfus	63.60	kJ/mol	Joback Method
hvap	96.45	kJ/mol	Joback Method
log10ws	-9.19		Crippen Method
logp	7.704		Crippen Method
mcvol	391.830	ml/mol	McGowan Method
pc	829.55	kPa	Joback Method
rinpol	2944.00		NIST Webbook
rinpol	2944.00		NIST Webbook
tb	1022.85	K	Joback Method
tc	1258.18	K	Joback Method
tf	581.93	K	Joback Method
vc	1.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1358.94	J/mol×K	1022.85	Joback Method
cpg	1376.67	J/mol×K	1062.07	Joback Method
cpg	1392.97	J/mol×K	1101.29	Joback Method
cpg	1407.95	J/mol×K	1140.51	Joback Method
cpg	1421.74	J/mol×K	1179.73	Joback Method
cpg	1434.47	J/mol×K	1218.96	Joback Method
cpg	1446.24	J/mol×K	1258.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346726&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