L-Valine, N-(3-methoxy-2,4,5-trifluorobenzoyl)-, tetradecyl ester

Inchi: InChI=1S/C27H42F3NO4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-35-27(33)24(19(2)3)31-
InchiKey: NCHVDNYYIYCGHT-UHFFFAOYSA-N
Formula: C27H42F3NO4
SMILES: CCCCCCCCCCCCCCOC(=O)C(NC(=O)c1cc(F)c(F)c(OC)c1F)C(C)C
Mol. weight [g/mol]: 501.62

Physical Properties

Property code	Value	Unit	Source
gf	-717.41	kJ/mol	Joback Method
hf	-1444.98	kJ/mol	Joback Method
hfus	71.04	kJ/mol	Joback Method
hvap	102.14	kJ/mol	Joback Method
log10ws	-9.20		Crippen Method
logp	7.111		Crippen Method
mcvol	397.700	ml/mol	McGowan Method
pc	792.15	kPa	Joback Method
rinpol	3159.00		NIST Webbook
rinpol	3159.00		NIST Webbook
tb	1063.44	K	Joback Method
tc	1319.59	K	Joback Method
tf	639.30	K	Joback Method
vc	1.565	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1384.39	J/mol×K	1063.44	Joback Method
cpg	1400.79	J/mol×K	1106.13	Joback Method
cpg	1414.98	J/mol×K	1148.82	Joback Method
cpg	1427.02	J/mol×K	1191.52	Joback Method
cpg	1436.98	J/mol×K	1234.21	Joback Method
cpg	1444.91	J/mol×K	1276.90	Joback Method
cpg	1450.89	J/mol×K	1319.59	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=U346438&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