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

Inchi: InChI=1S/C29H46F3NO4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-37-29(35)26(21(2
InchiKey: VNDCNVDCQWOKMQ-UHFFFAOYSA-N
Formula: C29H46F3NO4
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(NC(=O)c1cc(F)c(F)c(OC)c1F)C(C)C
Mol. weight [g/mol]: 529.67

Physical Properties

Property code	Value	Unit	Source
gf	-700.57	kJ/mol	Joback Method
hf	-1486.26	kJ/mol	Joback Method
hfus	76.22	kJ/mol	Joback Method
hvap	106.59	kJ/mol	Joback Method
log10ws	-10.04		Crippen Method
logp	7.891		Crippen Method
mcvol	425.880	ml/mol	McGowan Method
pc	713.01	kPa	Joback Method
rinpol	3366.00		NIST Webbook
rinpol	3366.00		NIST Webbook
tb	1109.20	K	Joback Method
tc	1392.49	K	Joback Method
tf	661.84	K	Joback Method
vc	1.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1509.43	J/mol×K	1109.20	Joback Method
cpg	1526.48	J/mol×K	1156.42	Joback Method
cpg	1540.81	J/mol×K	1203.63	Joback Method
cpg	1552.50	J/mol×K	1250.85	Joback Method
cpg	1561.66	J/mol×K	1298.06	Joback Method
cpg	1568.40	J/mol×K	1345.28	Joback Method
cpg	1572.80	J/mol×K	1392.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346440&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