L-Valine, N-(2,5-ditrifluoromethylbenzoyl)-, octadecyl ester

Inchi: InChI=1S/C32H49F6NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-42-30(41)28
InchiKey: BSAUAWZETINORS-UHFFFAOYSA-N
Formula: C32H49F6NO3
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(NC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F)C(C)C
Mol. weight [g/mol]: 609.73

Physical Properties

Property code	Value	Unit	Source
gf	-1129.80	kJ/mol	Joback Method
hf	-1998.85	kJ/mol	Joback Method
hfus	77.99	kJ/mol	Joback Method
hvap	104.49	kJ/mol	Joback Method
log10ws	-11.97		Crippen Method
logp	10.283		Crippen Method
mcvol	467.590	ml/mol	McGowan Method
pc	599.85	kPa	Joback Method
rinpol	3328.00		NIST Webbook
rinpol	3328.00		NIST Webbook
tb	1136.81	K	Joback Method
tc	1451.75	K	Joback Method
tf	654.99	K	Joback Method
vc	1.859	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1696.40	J/mol×K	1136.81	Joback Method
cpg	1719.28	J/mol×K	1189.30	Joback Method
cpg	1740.38	J/mol×K	1241.79	Joback Method
cpg	1760.09	J/mol×K	1294.28	Joback Method
cpg	1778.82	J/mol×K	1346.77	Joback Method
cpg	1796.95	J/mol×K	1399.26	Joback Method
cpg	1814.89	J/mol×K	1451.75	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=U346582&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