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

Inchi: InChI=1S/C31H50F3NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-23-38-30(37)28
InchiKey: JNXJWZYIMMLBIS-UHFFFAOYSA-N
Formula: C31H50F3NO3
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(NC(=O)c1cccc(C(F)(F)F)c1)C(C)C
Mol. weight [g/mol]: 541.73

Physical Properties

Property code	Value	Unit	Source
gf	-547.00	kJ/mol	Joback Method
hf	-1369.66	kJ/mol	Joback Method
hfus	73.96	kJ/mol	Joback Method
hvap	105.35	kJ/mol	Joback Method
log10ws	-10.86		Crippen Method
logp	9.265		Crippen Method
mcvol	448.190	ml/mol	McGowan Method
pc	672.55	kPa	Joback Method
rinpol	3355.00		NIST Webbook
rinpol	3355.00		NIST Webbook
tb	1114.37	K	Joback Method
tc	1396.68	K	Joback Method
tf	627.01	K	Joback Method
vc	1.760	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1613.58	J/mol×K	1114.37	Joback Method
cpg	1634.20	J/mol×K	1161.42	Joback Method
cpg	1652.97	J/mol×K	1208.47	Joback Method
cpg	1670.13	J/mol×K	1255.52	Joback Method
cpg	1685.92	J/mol×K	1302.57	Joback Method
cpg	1700.58	J/mol×K	1349.63	Joback Method
cpg	1714.35	J/mol×K	1396.68	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346730&Units=SI

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