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

Inchi: InChI=1S/C32H52F3NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-24-39-31(38
InchiKey: RHZTWHIKOHFLOR-UHFFFAOYSA-N
Formula: C32H52F3NO3
SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)C(NC(=O)c1cccc(C(F)(F)F)c1)C(C)C
Mol. weight [g/mol]: 555.76

Physical Properties

Property code	Value	Unit	Source
gf	-538.58	kJ/mol	Joback Method
hf	-1390.30	kJ/mol	Joback Method
hfus	76.55	kJ/mol	Joback Method
hvap	107.58	kJ/mol	Joback Method
log10ws	-11.28		Crippen Method
logp	9.655		Crippen Method
mcvol	462.280	ml/mol	McGowan Method
pc	640.27	kPa	Joback Method
rinpol	3456.00		NIST Webbook
rinpol	3456.00		NIST Webbook
tb	1137.25	K	Joback Method
tc	1435.35	K	Joback Method
tf	638.28	K	Joback Method
vc	1.815	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1678.13	J/mol×K	1137.25	Joback Method
cpg	1699.70	J/mol×K	1186.93	Joback Method
cpg	1719.30	J/mol×K	1236.62	Joback Method
cpg	1737.21	J/mol×K	1286.30	Joback Method
cpg	1753.72	J/mol×K	1335.99	Joback Method
cpg	1769.14	J/mol×K	1385.67	Joback Method
cpg	1783.74	J/mol×K	1435.35	Joback Method

Sources

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=U346731&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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