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

Inchi: InChI=1S/C33H54F3NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-25-40-32

InchiKey: IUDXNGYYPYOTSV-UHFFFAOYSA-N

Formula: C33H54F3NO3

SMILES: CCCCCCCCCCCCCCCCCCCCCOC(=O)C(NC(=O)c1cccc(C(F)(F)F)c1)C(C)C

Mol. weight [g/mol]: 569.78

Physical Properties

Property code	Value	Unit	Source
gf	-530.16	kJ/mol	Joback Method
hf	-1410.94	kJ/mol	Joback Method
hfus	79.14	kJ/mol	Joback Method
hvap	109.80	kJ/mol	Joback Method
log10ws	-11.70		Crippen Method
logp	10.045		Crippen Method
mcvol	476.370	ml/mol	McGowan Method
pc	610.27	kPa	Joback Method
rinpol	3569.00		NIST Webbook
tb	1160.13	K	Joback Method
tc	1475.92	K	Joback Method
tf	649.55	K	Joback Method
vc	1.871	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1742.99	J/mol×K	1160.13	Joback Method
cpg	1765.63	J/mol×K	1212.76	Joback Method
cpg	1786.17	J/mol×K	1265.39	Joback Method
cpg	1804.94	J/mol×K	1318.02	Joback Method
cpg	1822.32	J/mol×K	1370.65	Joback Method
cpg	1838.66	J/mol×K	1423.28	Joback Method
cpg	1854.32	J/mol×K	1475.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346732&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