L-Valine, N-(2-trifluoromethylbenzoyl)-, tridecyl ester

Inchi: InChI=1S/C26H40F3NO3/c1-4-5-6-7-8-9-10-11-12-13-16-19-33-25(32)23(20(2)3)30-24(3

InchiKey: ZMQOCBFUKKWZCB-UHFFFAOYSA-N

Formula: C26H40F3NO3

SMILES: CCCCCCCCCCCCCOC(=O)C(NC(=O)c1ccccc1C(F)(F)F)C(C)C

Mol. weight [g/mol]: 471.60

Physical Properties

Property code	Value	Unit	Source
gf	-589.10	kJ/mol	Joback Method
hf	-1266.46	kJ/mol	Joback Method
hfus	61.01	kJ/mol	Joback Method
hvap	94.22	kJ/mol	Joback Method
log10ws	-8.77		Crippen Method
logp	7.314		Crippen Method
mcvol	377.740	ml/mol	McGowan Method
pc	877.39	kPa	Joback Method
rinpol	2928.00		NIST Webbook
rinpol	2928.00		NIST Webbook
tb	999.97	K	Joback Method
tc	1227.03	K	Joback Method
tf	570.66	K	Joback Method
vc	1.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1296.30	J/mol×K	999.97	Joback Method
cpg	1313.49	J/mol×K	1037.81	Joback Method
cpg	1329.33	J/mol×K	1075.66	Joback Method
cpg	1343.91	J/mol×K	1113.50	Joback Method
cpg	1357.36	J/mol×K	1151.35	Joback Method
cpg	1369.76	J/mol×K	1189.19	Joback Method
cpg	1381.23	J/mol×K	1227.03	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=U346713&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