L-Valine, N-(4-fluoro-2-trifluoromethylbenzoyl)-, undecyl ester

Inchi: InChI=1S/C24H35F4NO3/c1-4-5-6-7-8-9-10-11-12-15-32-23(31)21(17(2)3)29-22(30)19-1
InchiKey: VJZVDUCLMVIJIC-UHFFFAOYSA-N
Formula: C24H35F4NO3
SMILES: CCCCCCCCCCCOC(=O)C(NC(=O)c1ccc(F)cc1C(F)(F)F)C(C)C
Mol. weight [g/mol]: 461.53

Physical Properties

Property code	Value	Unit	Source
gf	-810.38	kJ/mol	Joback Method
hf	-1432.76	kJ/mol	Joback Method
hfus	58.52	kJ/mol	Joback Method
hvap	89.62	kJ/mol	Joback Method
log10ws	-8.26		Crippen Method
logp	6.673		Crippen Method
mcvol	351.330	ml/mol	McGowan Method
pc	950.25	kPa	Joback Method
rinpol	2639.00		NIST Webbook
rinpol	2639.00		NIST Webbook
tb	958.46	K	Joback Method
tc	1174.15	K	Joback Method
tf	561.23	K	Joback Method
vc	1.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1178.66	J/mol×K	958.46	Joback Method
cpg	1194.77	J/mol×K	994.41	Joback Method
cpg	1209.63	J/mol×K	1030.36	Joback Method
cpg	1223.31	J/mol×K	1066.31	Joback Method
cpg	1235.90	J/mol×K	1102.25	Joback Method
cpg	1247.47	J/mol×K	1138.20	Joback Method
cpg	1258.10	J/mol×K	1174.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346487&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

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