L-Valine, N-(2,5-ditrifluoromethylbenzoyl)-, undecyl ester

Inchi: InChI=1S/C25H35F6NO3/c1-4-5-6-7-8-9-10-11-12-15-35-23(34)21(17(2)3)32-22(33)19-1

InchiKey: QCXLUXFSOLGWGQ-UHFFFAOYSA-N

Formula: C25H35F6NO3

SMILES: CCCCCCCCCCCOC(=O)C(NC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F)C(C)C

Mol. weight [g/mol]: 511.54

Physical Properties

Property code	Value	Unit	Source
gf	-1188.74	kJ/mol	Joback Method
hf	-1854.37	kJ/mol	Joback Method
hfus	59.86	kJ/mol	Joback Method
hvap	88.91	kJ/mol	Joback Method
log10ws	-9.04		Crippen Method
logp	7.553		Crippen Method
mcvol	368.960	ml/mol	McGowan Method
pc	859.48	kPa	Joback Method
rinpol	2534.00		NIST Webbook
rinpol	2534.00		NIST Webbook
tb	976.65	K	Joback Method
tc	1199.57	K	Joback Method
tf	576.10	K	Joback Method
vc	1.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1253.92	J/mol×K	976.65	Joback Method
cpg	1270.30	J/mol×K	1013.80	Joback Method
cpg	1285.47	J/mol×K	1050.96	Joback Method
cpg	1299.54	J/mol×K	1088.11	Joback Method
cpg	1312.64	J/mol×K	1125.27	Joback Method
cpg	1324.87	J/mol×K	1162.42	Joback Method
cpg	1336.36	J/mol×K	1199.57	Joback Method

Sources

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=U346576&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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