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

Inchi: InChI=1S/C28H41F6NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-18-38-26(37)24(20(2)3)35-2

InchiKey: KLGHBCSQONRHHD-UHFFFAOYSA-N

Formula: C28H41F6NO3

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

Mol. weight [g/mol]: 553.62

Physical Properties

Property code	Value	Unit	Source
gf	-1163.48	kJ/mol	Joback Method
hf	-1916.29	kJ/mol	Joback Method
hfus	67.63	kJ/mol	Joback Method
hvap	95.59	kJ/mol	Joback Method
log10ws	-10.29		Crippen Method
logp	8.723		Crippen Method
mcvol	411.230	ml/mol	McGowan Method
pc	730.86	kPa	Joback Method
rinpol	2810.00		NIST Webbook
rinpol	2810.00		NIST Webbook
tb	1045.29	K	Joback Method
tc	1298.30	K	Joback Method
tf	609.91	K	Joback Method
vc	1.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1440.86	J/mol×K	1045.29	Joback Method
cpg	1459.42	J/mol×K	1087.46	Joback Method
cpg	1476.54	J/mol×K	1129.63	Joback Method
cpg	1492.43	J/mol×K	1171.80	Joback Method
cpg	1507.25	J/mol×K	1213.96	Joback Method
cpg	1521.20	J/mol×K	1256.13	Joback Method
cpg	1534.45	J/mol×K	1298.30	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=U346578&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