L-Valine, N-(2,6-difluoro-3-methylbenzoyl)-, tetradecyl ester

Inchi: InChI=1S/C27H43F2NO3/c1-5-6-7-8-9-10-11-12-13-14-15-16-19-33-27(32)25(20(2)3)30-
InchiKey: IDHXZKHJQHUSEF-UHFFFAOYSA-N
Formula: C27H43F2NO3
SMILES: CCCCCCCCCCCCCCOC(=O)C(NC(=O)c1c(F)ccc(C)c1F)C(C)C
Mol. weight [g/mol]: 467.63

Physical Properties

Property code	Value	Unit	Source
gf	-407.97	kJ/mol	Joback Method
hf	-1105.18	kJ/mol	Joback Method
hfus	67.16	kJ/mol	Joback Method
hvap	99.89	kJ/mol	Joback Method
log10ws	-9.22		Crippen Method
logp	7.272		Crippen Method
mcvol	390.060	ml/mol	McGowan Method
pc	827.64	kPa	Joback Method
rinpol	3200.00		NIST Webbook
rinpol	3200.00		NIST Webbook
tb	1036.77	K	Joback Method
tc	1277.07	K	Joback Method
tf	603.96	K	Joback Method
vc	1.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1350.92	J/mol×K	1036.77	Joback Method
cpg	1368.40	J/mol×K	1076.82	Joback Method
cpg	1384.14	J/mol×K	1116.87	Joback Method
cpg	1398.23	J/mol×K	1156.92	Joback Method
cpg	1410.75	J/mol×K	1196.97	Joback Method
cpg	1421.78	J/mol×K	1237.02	Joback Method
cpg	1431.39	J/mol×K	1277.07	Joback Method

Sources

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=U346452&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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