L-Valine, N-(2-fluoro-5-trifluoromethylbenzoyl)-, tetradecyl ester

Inchi: InChI=1S/C27H41F4NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-18-35-26(34)24(20(2)3)32-2
InchiKey: PJCQCMFHVKLWEO-UHFFFAOYSA-N
Formula: C27H41F4NO3
SMILES: CCCCCCCCCCCCCCOC(=O)C(NC(=O)c1cc(C(F)(F)F)ccc1F)C(C)C
Mol. weight [g/mol]: 503.61

Physical Properties

Property code	Value	Unit	Source
gf	-785.12	kJ/mol	Joback Method
hf	-1494.68	kJ/mol	Joback Method
hfus	66.29	kJ/mol	Joback Method
hvap	96.29	kJ/mol	Joback Method
log10ws	-9.52		Crippen Method
logp	7.843		Crippen Method
mcvol	393.600	ml/mol	McGowan Method
pc	801.60	kPa	Joback Method
rinpol	2922.00		NIST Webbook
rinpol	2922.00		NIST Webbook
tb	1027.10	K	Joback Method
tc	1267.19	K	Joback Method
tf	595.04	K	Joback Method
vc	1.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1364.84	J/mol×K	1027.10	Joback Method
cpg	1382.55	J/mol×K	1067.11	Joback Method
cpg	1398.74	J/mol×K	1107.13	Joback Method
cpg	1413.54	J/mol×K	1147.14	Joback Method
cpg	1427.07	J/mol×K	1187.16	Joback Method
cpg	1439.46	J/mol×K	1227.17	Joback Method
cpg	1450.82	J/mol×K	1267.19	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=U346522&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