L-Valine, N-(3-methoxy-2,4,5-trifluorobenzoyl)-, dodecyl ester

Inchi: InChI=1S/C25H38F3NO4/c1-5-6-7-8-9-10-11-12-13-14-15-33-25(31)22(17(2)3)29-24(30)
InchiKey: GCTDMCPOYFJXJU-UHFFFAOYSA-N
Formula: C25H38F3NO4
SMILES: CCCCCCCCCCCCOC(=O)C(N=C(O)c1cc(F)c(F)c(OC)c1F)C(C)C
Mol. weight [g/mol]: 473.57

Physical Properties

Property code	Value	Unit	Source
hf	-1424.39	kJ/mol	Joback Method
hvap	104.58	kJ/mol	Joback Method
log10ws	-7.90		Crippen Method
logp	6.906		Crippen Method
mcvol	369.520	ml/mol	McGowan Method
pc	842.60	kPa	Joback Method
rinpol	2946.00		NIST Webbook
rinpol	2946.00		NIST Webbook
tb	1082.38	K	Joback Method
tc	1345.25	K	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346437&Units=SI

Legend

hf: Enthalpy of formation 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