L-Valine, N-(2-methoxybenzoyl)-, pentadecyl ester

Inchi: InChI=1S/C28H47NO4/c1-5-6-7-8-9-10-11-12-13-14-15-16-19-22-33-28(31)26(23(2)3)29

InchiKey: JHDIHFWSAICUHV-UHFFFAOYSA-N

Formula: C28H47NO4

SMILES: CCCCCCCCCCCCCCCOC(=O)C(N=C(O)c1ccccc1OC)C(C)C

Mol. weight [g/mol]: 461.68

Physical Properties

Property code	Value	Unit	Source
hf	-863.57	kJ/mol	Joback Method
hvap	111.72	kJ/mol	Joback Method
log10ws	-8.17		Crippen Method
logp	7.659		Crippen Method
mcvol	406.480	ml/mol	McGowan Method
pc	792.15	kPa	Joback Method
rinpol	3449.00		NIST Webbook
rinpol	3449.00		NIST Webbook
tb	1138.27	K	Joback Method
tc	1416.74	K	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=U346599&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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