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

Inchi: InChI=1S/C27H45NO4/c1-5-6-7-8-9-10-11-12-13-14-15-18-21-32-27(30)25(22(2)3)28-26

InchiKey: SGVAVDMLAYJNGH-UHFFFAOYSA-N

Formula: C27H45NO4

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

Mol. weight [g/mol]: 447.65

Physical Properties

Property code	Value	Unit	Source
hf	-842.93	kJ/mol	Joback Method
hvap	109.50	kJ/mol	Joback Method
log10ws	-7.75		Crippen Method
logp	7.269		Crippen Method
mcvol	392.390	ml/mol	McGowan Method
pc	836.76	kPa	Joback Method
rinpol	3334.00		NIST Webbook
rinpol	3334.00		NIST Webbook
tb	1115.39	K	Joback Method
tc	1381.36	K	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=U346598&Units=SI

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

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

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