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

Inchi: InChI=1S/C25H41NO4/c1-5-6-7-8-9-10-11-12-13-16-19-30-25(28)23(20(2)3)26-24(27)21
InchiKey: YNDKIERMGKYAGX-UHFFFAOYSA-N
Formula: C25H41NO4
SMILES: CCCCCCCCCCCCOC(=O)C(N=C(O)c1ccccc1OC)C(C)C
Mol. weight [g/mol]: 419.60

Physical Properties

Property code	Value	Unit	Source
hf	-801.65	kJ/mol	Joback Method
hvap	105.04	kJ/mol	Joback Method
log10ws	-6.91		Crippen Method
logp	6.489		Crippen Method
mcvol	364.210	ml/mol	McGowan Method
pc	938.07	kPa	Joback Method
rinpol	3125.00		NIST Webbook
rinpol	3125.00		NIST Webbook
tb	1069.63	K	Joback Method
tc	1315.11	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=U346597&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