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

Inchi: InChI=1S/C23H37NO4/c1-5-6-7-8-9-10-11-14-17-28-23(26)21(18(2)3)24-22(25)19-15-12
InchiKey: IVKGDWVGBYJTRL-UHFFFAOYSA-N
Formula: C23H37NO4
SMILES: CCCCCCCCCCOC(=O)C(N=C(O)c1ccccc1OC)C(C)C
Mol. weight [g/mol]: 391.54

Physical Properties

Property code	Value	Unit	Source
hf	-760.37	kJ/mol	Joback Method
hvap	100.59	kJ/mol	Joback Method
log10ws	-6.07		Crippen Method
logp	5.708		Crippen Method
mcvol	336.030	ml/mol	McGowan Method
pc	1058.95	kPa	Joback Method
rinpol	2897.00		NIST Webbook
rinpol	2897.00		NIST Webbook
tb	1023.87	K	Joback Method
tc	1254.19	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=U346595&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