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

Inchi: InChI=1S/C18H27NO4/c1-5-6-9-12-23-18(21)16(13(2)3)19-17(20)14-10-7-8-11-15(14)22
InchiKey: RHMMGDGDKLRIKH-UHFFFAOYSA-N
Formula: C18H27NO4
SMILES: CCCCCOC(=O)C(N=C(O)c1ccccc1OC)C(C)C
Mol. weight [g/mol]: 321.41

Physical Properties

Property code	Value	Unit	Source
hf	-657.17	kJ/mol	Joback Method
hvap	89.46	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.758		Crippen Method
mcvol	265.580	ml/mol	McGowan Method
pc	1487.29	kPa	Joback Method
rinpol	2402.00		NIST Webbook
rinpol	2402.00		NIST Webbook
tb	909.47	K	Joback Method
tc	1120.84	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=U346592&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