L-Valine, N-(3-phenylpropionyl)-, octyl ester

Inchi: InChI=1S/C22H35NO3/c1-4-5-6-7-8-12-17-26-22(25)21(18(2)3)23-20(24)16-15-19-13-10
InchiKey: MALOLHZJIKAMLG-UHFFFAOYSA-N
Formula: C22H35NO3
SMILES: CCCCCCCCOC(=O)C(N=C(O)CCc1ccccc1)C(C)C
Mol. weight [g/mol]: 361.52

Physical Properties

Property code	Value	Unit	Source
hf	-596.04	kJ/mol	Joback Method
hvap	95.29	kJ/mol	Joback Method
log10ws	-5.85		Crippen Method
logp	5.504		Crippen Method
mcvol	316.070	ml/mol	McGowan Method
pc	1153.00	kPa	Joback Method
rinpol	2667.00		NIST Webbook
rinpol	2667.00		NIST Webbook
tb	973.59	K	Joback Method
tc	1192.32	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=U346081&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