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

Inchi: InChI=1S/C21H33NO3/c1-4-5-6-7-11-16-25-21(24)20(17(2)3)22-19(23)15-14-18-12-9-8-
InchiKey: RXPPSSNUBHLGIK-UHFFFAOYSA-N
Formula: C21H33NO3
SMILES: CCCCCCCOC(=O)C(N=C(O)CCc1ccccc1)C(C)C
Mol. weight [g/mol]: 347.49

Physical Properties

Property code	Value	Unit	Source
hf	-575.40	kJ/mol	Joback Method
hvap	93.07	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	5.114		Crippen Method
mcvol	301.980	ml/mol	McGowan Method
pc	1232.01	kPa	Joback Method
rinpol	2567.00		NIST Webbook
rinpol	2567.00		NIST Webbook
tb	950.71	K	Joback Method
tc	1165.66	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346080&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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