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

Inchi: InChI=1S/C19H29NO3/c1-4-5-9-14-23-19(22)18(15(2)3)20-17(21)13-12-16-10-7-6-8-11-
InchiKey: QMXKQAMCSADTHI-UHFFFAOYSA-N
Formula: C19H29NO3
SMILES: CCCCCOC(=O)C(N=C(O)CCc1ccccc1)C(C)C
Mol. weight [g/mol]: 319.44

Physical Properties

Property code	Value	Unit	Source
hf	-534.12	kJ/mol	Joback Method
hvap	88.62	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	4.334		Crippen Method
mcvol	273.800	ml/mol	McGowan Method
pc	1416.50	kPa	Joback Method
rinpol	2364.00		NIST Webbook
rinpol	2364.00		NIST Webbook
tb	904.95	K	Joback Method
tc	1115.11	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346078&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