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

Inchi: InChI=1S/C20H31NO3/c1-4-5-6-10-15-24-20(23)19(16(2)3)21-18(22)14-13-17-11-8-7-9-
InchiKey: XPEPTRGJXJNZIG-UHFFFAOYSA-N
Formula: C20H31NO3
SMILES: CCCCCCOC(=O)C(N=C(O)CCc1ccccc1)C(C)C
Mol. weight [g/mol]: 333.46

Physical Properties

Property code	Value	Unit	Source
hf	-554.76	kJ/mol	Joback Method
hvap	90.84	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.724		Crippen Method
mcvol	287.890	ml/mol	McGowan Method
pc	1319.43	kPa	Joback Method
rinpol	2465.00		NIST Webbook
rinpol	2465.00		NIST Webbook
tb	927.83	K	Joback Method
tc	1139.95	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346079&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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