L-Norvaline, N-((1R)-(-)-menthyloxycarbonyl)-, hexyl ester

Inchi: InChI=1S/C22H41NO4/c1-6-8-9-10-14-26-21(24)19(11-7-2)23-22(25)27-20-15-17(5)12-1

InchiKey: YJRMRKYOWOUMJI-UHFFFAOYSA-N

Formula: C22H41NO4

SMILES: CCCCCCOC(=O)C(CCC)N=C(O)OC1CC(C)CCC1C(C)C

Mol. weight [g/mol]: 383.57

Physical Properties

Property code	Value	Unit	Source
hf	-951.15	kJ/mol	Joback Method
hvap	95.24	kJ/mol	Joback Method
log10ws	-5.85		Crippen Method
logp	5.670		Crippen Method
mcvol	334.840	ml/mol	McGowan Method
pc	1005.26	kPa	Joback Method
rinpol	2458.00		NIST Webbook
rinpol	2458.00		NIST Webbook
tb	979.54	K	Joback Method
tc	1199.24	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U392879&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