L-Norvaline, N-octyloxycarbonyl-, hexyl ester

Inchi: InChI=1S/C20H39NO4/c1-4-7-9-11-12-14-17-25-20(23)21-18(15-6-3)19(22)24-16-13-10-
InchiKey: WAJVNFZXWCUBEE-GOSISDBHSA-N
Formula: C20H39NO4
SMILES: CCCCCCCCOC(O)=NC(CCC)C(=O)OCCCCCC
Mol. weight [g/mol]: 357.53

Physical Properties

Property code	Value	Unit	Source
hf	-918.23	kJ/mol	Joback Method
hvap	91.36	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	5.570		Crippen Method
mcvol	317.520	ml/mol	McGowan Method
pc	1034.57	kPa	Joback Method
rinpol	2387.00		NIST Webbook
rinpol	2387.00		NIST Webbook
tb	924.01	K	Joback Method
tc	1132.03	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U392846&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