l-Norvaline, N-allyloxycarbonyl-, octyl ester

Inchi: InChI=1S/C17H31NO4/c1-4-7-8-9-10-11-14-21-16(19)15(12-5-2)18-17(20)22-13-6-3/h6,1
InchiKey: WPOZNBKUDJCGDA-UHFFFAOYSA-N
Formula: C17H31NO4
SMILES: C=CCOC(O)=NC(CCC)C(=O)OCCCCCCCC
Mol. weight [g/mol]: 313.43

Physical Properties

Property code	Value	Unit	Source
hf	-730.88	kJ/mol	Joback Method
hvap	84.02	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	4.175		Crippen Method
mcvol	270.950	ml/mol	McGowan Method
pc	1294.86	kPa	Joback Method
rinpol	1919.00		NIST Webbook
rinpol	1919.00		NIST Webbook
tb	852.05	K	Joback Method
tc	1045.38	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U320748&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