L-Norvaline, N-(but-3-en-1-yloxycarbonyl)-, pentyl ester

Inchi: InChI=1S/C15H27NO4/c1-4-7-9-12-19-14(17)13(10-6-3)16-15(18)20-11-8-5-2/h5,13H,2,4

InchiKey: VWICRYQOIDTEQD-CYBMUJFWSA-N

Formula: C15H27NO4

SMILES: C=CCCOC(O)=NC(CCC)C(=O)OCCCCC

Mol. weight [g/mol]: 285.38

Physical Properties

Property code	Value	Unit	Source
hf	-689.60	kJ/mol	Joback Method
hvap	79.56	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	3.395		Crippen Method
mcvol	242.770	ml/mol	McGowan Method
pc	1494.19	kPa	Joback Method
rinpol	1891.00		NIST Webbook
rinpol	1891.00		NIST Webbook
tb	806.29	K	Joback Method
tc	994.84	K	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U392868&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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