L-Valine, N-(3-methylbut-2-enoyl)-, undecyl ester

Inchi: InChI=1S/C21H39NO3/c1-6-7-8-9-10-11-12-13-14-15-25-21(24)20(18(4)5)22-19(23)16-1

InchiKey: ZQOMAZTXTZWBCG-UHFFFAOYSA-N

Formula: C21H39NO3

SMILES: CCCCCCCCCCCOC(=O)C(N=C(O)C=C(C)C)C(C)C

Mol. weight [g/mol]: 353.54

Physical Properties

Property code	Value	Unit	Source
hf	-704.50	kJ/mol	Joback Method
hvap	90.83	kJ/mol	Joback Method
log10ws	-6.18		Crippen Method
logp	6.008		Crippen Method
mcvol	321.440	ml/mol	McGowan Method
pc	1025.31	kPa	Joback Method
rinpol	2480.00		NIST Webbook
rinpol	2480.00		NIST Webbook
tb	928.07	K	Joback Method
tc	1136.22	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346076&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