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

Inchi: InChI=1S/C15H27NO3/c1-6-7-8-9-19-15(18)14(12(4)5)16-13(17)10-11(2)3/h10,12,14H,6
InchiKey: WXYZMYGLZXHHNJ-UHFFFAOYSA-N
Formula: C15H27NO3
SMILES: CCCCCOC(=O)C(N=C(O)C=C(C)C)C(C)C
Mol. weight [g/mol]: 269.38

Physical Properties

Property code	Value	Unit	Source
hf	-580.66	kJ/mol	Joback Method
hvap	77.48	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.667		Crippen Method
mcvol	236.900	ml/mol	McGowan Method
pc	1541.49	kPa	Joback Method
rinpol	1893.00		NIST Webbook
rinpol	1893.00		NIST Webbook
tb	790.79	K	Joback Method
tc	983.50	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346066&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

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