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

Inchi: InChI=1S/C19H35NO3/c1-6-7-8-9-10-11-12-13-23-19(22)18(16(4)5)20-17(21)14-15(2)3/h
InchiKey: UATMBZVQRUPTHJ-UHFFFAOYSA-N
Formula: C19H35NO3
SMILES: CCCCCCCCCOC(=O)C(N=C(O)C=C(C)C)C(C)C
Mol. weight [g/mol]: 325.49

Physical Properties

Property code	Value	Unit	Source
hf	-663.22	kJ/mol	Joback Method
hvap	86.38	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	5.228		Crippen Method
mcvol	293.260	ml/mol	McGowan Method
pc	1164.04	kPa	Joback Method
rinpol	2279.00		NIST Webbook
rinpol	2279.00		NIST Webbook
tb	882.31	K	Joback Method
tc	1082.04	K	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346073&Units=SI

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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