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

Inchi: InChI=1S/C20H37NO3/c1-6-7-8-9-10-11-12-13-14-24-20(23)19(17(4)5)21-18(22)15-16(2
InchiKey: JUSABVAYSUUWME-UHFFFAOYSA-N
Formula: C20H37NO3
SMILES: CCCCCCCCCCOC(=O)C(N=C(O)C=C(C)C)C(C)C
Mol. weight [g/mol]: 339.51

Physical Properties

Property code	Value	Unit	Source
hf	-683.86	kJ/mol	Joback Method
hvap	88.60	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	5.618		Crippen Method
mcvol	307.350	ml/mol	McGowan Method
pc	1091.38	kPa	Joback Method
rinpol	2382.00		NIST Webbook
rinpol	2382.00		NIST Webbook
tb	905.19	K	Joback Method
tc	1108.67	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=U346074&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