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

Inchi: InChI=1S/C12H21NO3/c1-6-16-12(15)11(9(4)5)13-10(14)7-8(2)3/h7,9,11H,6H2,1-5H3,(H

InchiKey: TVLWZBOYAZKPOJ-UHFFFAOYSA-N

Formula: C12H21NO3

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

Mol. weight [g/mol]: 227.30

Physical Properties

Property code	Value	Unit	Source
hf	-518.74	kJ/mol	Joback Method
hvap	70.80	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	2.497		Crippen Method
mcvol	194.630	ml/mol	McGowan Method
pc	1959.60	kPa	Joback Method
rinpol	1608.00		NIST Webbook
rinpol	1608.00		NIST Webbook
tb	722.15	K	Joback Method
tc	916.39	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=U346063&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