l-Valine, N-caproyl-, methyl ester

Inchi: InChI=1S/C12H23NO3/c1-5-6-7-8-10(14)13-11(9(2)3)12(15)16-4/h9,11H,5-8H2,1-4H3,(H
InchiKey: XFEUHQYGLOQDDX-UHFFFAOYSA-N
Formula: C12H23NO3
SMILES: CCCCCC(O)=NC(C(=O)OC)C(C)C
Mol. weight [g/mol]: 229.32

Physical Properties

Property code	Value	Unit	Source
hf	-626.17	kJ/mol	Joback Method
hvap	70.76	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	2.721		Crippen Method
mcvol	198.930	ml/mol	McGowan Method
pc	1864.33	kPa	Joback Method
rinpol	1568.00		NIST Webbook
rinpol	1568.00		NIST Webbook
tb	718.11	K	Joback Method
tc	904.62	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U299733&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