l-Valine, N-capryloyl-, methyl ester

Inchi: InChI=1S/C14H27NO3/c1-5-6-7-8-9-10-12(16)15-13(11(2)3)14(17)18-4/h11,13H,5-10H2
InchiKey: BBEXIDMPTFADQN-UHFFFAOYSA-N
Formula: C14H27NO3
SMILES: CCCCCCCC(=O)NC(C(=O)OC)C(C)C
Mol. weight [g/mol]: 257.37

Physical Properties

Property code	Value	Unit	Source
gf	-211.33	kJ/mol	Joback Method
hf	-646.76	kJ/mol	Joback Method
hfus	34.45	kJ/mol	Joback Method
hvap	68.32	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	2.661		Crippen Method
mcvol	227.110	ml/mol	McGowan Method
pc	1701.90	kPa	Joback Method
rinpol	1770.00		NIST Webbook
tb	699.17	K	Joback Method
tc	882.83	K	Joback Method
tf	392.29	K	Joback Method
vc	0.873	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.04	J/mol×K	699.17	Joback Method
cpg	669.05	J/mol×K	729.78	Joback Method
cpg	684.22	J/mol×K	760.39	Joback Method
cpg	698.58	J/mol×K	791.00	Joback Method
cpg	712.14	J/mol×K	821.61	Joback Method
cpg	724.92	J/mol×K	852.22	Joback Method
cpg	736.93	J/mol×K	882.83	Joback Method

Sources

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=U299724&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point
vc:	Critical Volume