l-Leucine, N-caproyl-, methyl ester

Inchi: InChI=1S/C13H25NO3/c1-5-6-7-8-12(15)14-11(9-10(2)3)13(16)17-4/h10-11H,5-9H2,1-4H
InchiKey: DOCFZUAGCWOUJX-UHFFFAOYSA-N
Formula: C13H25NO3
SMILES: CCCCCC(=O)NC(CC(C)C)C(=O)OC
Mol. weight [g/mol]: 243.34

Physical Properties

Property code	Value	Unit	Source
gf	-219.75	kJ/mol	Joback Method
hf	-626.12	kJ/mol	Joback Method
hfus	31.86	kJ/mol	Joback Method
hvap	66.09	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	2.271		Crippen Method
mcvol	213.020	ml/mol	McGowan Method
pc	1845.16	kPa	Joback Method
rinpol	1641.00		NIST Webbook
rinpol	1641.00		NIST Webbook
tb	676.29	K	Joback Method
tc	860.80	K	Joback Method
tf	381.02	K	Joback Method
vc	0.817	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.39	J/mol×K	676.29	Joback Method
cpg	613.97	J/mol×K	707.04	Joback Method
cpg	628.75	J/mol×K	737.79	Joback Method
cpg	642.75	J/mol×K	768.54	Joback Method
cpg	655.99	J/mol×K	799.30	Joback Method
cpg	668.47	J/mol×K	830.05	Joback Method
cpg	680.21	J/mol×K	860.80	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=U299734&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