l-Leucine, N-capryloyl-, methyl ester

Inchi: InChI=1S/C15H29NO3/c1-5-6-7-8-9-10-14(17)16-13(11-12(2)3)15(18)19-4/h12-13H,5-11
InchiKey: ZRLCRYKBMRBAFD-UHFFFAOYSA-N
Formula: C15H29NO3
SMILES: CCCCCCCC(=O)NC(CC(C)C)C(=O)OC
Mol. weight [g/mol]: 271.40

Physical Properties

Property code	Value	Unit	Source
gf	-202.91	kJ/mol	Joback Method
hf	-667.40	kJ/mol	Joback Method
hfus	37.04	kJ/mol	Joback Method
hvap	70.55	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.051		Crippen Method
mcvol	241.200	ml/mol	McGowan Method
pc	1574.70	kPa	Joback Method
rinpol	1840.00		NIST Webbook
rinpol	1840.00		NIST Webbook
tb	722.05	K	Joback Method
tc	905.31	K	Joback Method
tf	403.56	K	Joback Method
vc	0.928	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	708.89	J/mol×K	722.05	Joback Method
cpg	725.28	J/mol×K	752.59	Joback Method
cpg	740.81	J/mol×K	783.14	Joback Method
cpg	755.49	J/mol×K	813.68	Joback Method
cpg	769.34	J/mol×K	844.23	Joback Method
cpg	782.37	J/mol×K	874.77	Joback Method
cpg	794.61	J/mol×K	905.31	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299725&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

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