L-Leucine, N-methyl-N-(but-3-yn-1-yloxycarbonyl)-, hexyl ester

Inchi: InChI=1S/C18H31NO4/c1-6-8-10-11-13-22-17(20)16(14-15(3)4)19(5)18(21)23-12-9-7-2/h
InchiKey: PJQBFQKBOBGHGT-MRXNPFEDSA-N
Formula: C18H31NO4
SMILES: C#CCCOC(=O)N(C)C(CC(C)C)C(=O)OCCCCCC
Mol. weight [g/mol]: 325.44

Physical Properties

Property code	Value	Unit	Source
gf	-38.19	kJ/mol	Joback Method
hf	-555.58	kJ/mol	Joback Method
hfus	46.90	kJ/mol	Joback Method
hvap	75.10	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.616		Crippen Method
mcvol	280.740	ml/mol	McGowan Method
pc	1379.91	kPa	Joback Method
rinpol	1972.00		NIST Webbook
rinpol	1972.00		NIST Webbook
tb	765.50	K	Joback Method
tc	951.51	K	Joback Method
tf	486.38	K	Joback Method
vc	1.060	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	839.48	J/mol×K	765.50	Joback Method
cpg	856.37	J/mol×K	796.50	Joback Method
cpg	872.30	J/mol×K	827.50	Joback Method
cpg	887.28	J/mol×K	858.51	Joback Method
cpg	901.36	J/mol×K	889.51	Joback Method
cpg	914.54	J/mol×K	920.51	Joback Method
cpg	926.85	J/mol×K	951.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392376&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