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

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

Physical Properties

Property code	Value	Unit	Source
gf	-40.63	kJ/mol	Joback Method
hf	-560.86	kJ/mol	Joback Method
hfus	43.38	kJ/mol	Joback Method
hvap	74.71	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.472		Crippen Method
mcvol	280.740	ml/mol	McGowan Method
pc	1388.15	kPa	Joback Method
rinpol	1934.00		NIST Webbook
rinpol	1934.00		NIST Webbook
tb	765.06	K	Joback Method
tc	952.95	K	Joback Method
tf	471.38	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	839.98	J/mol×K	765.06	Joback Method
cpg	857.05	J/mol×K	796.37	Joback Method
cpg	873.13	J/mol×K	827.69	Joback Method
cpg	888.24	J/mol×K	859.00	Joback Method
cpg	902.41	J/mol×K	890.32	Joback Method
cpg	915.67	J/mol×K	921.63	Joback Method
cpg	928.02	J/mol×K	952.95	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392387&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