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

Inchi: InChI=1S/C17H29NO4/c1-6-8-10-12-21-16(19)15(13-14(3)4)18(5)17(20)22-11-9-7-2/h2,1

InchiKey: RSEBXXQYWPFRKH-OAHLLOKOSA-N

Formula: C17H29NO4

SMILES: C#CCCOC(=O)N(C)C(CC(C)C)C(=O)OCCCCC

Mol. weight [g/mol]: 311.42

Physical Properties

Property code	Value	Unit	Source
gf	-46.61	kJ/mol	Joback Method
hf	-534.94	kJ/mol	Joback Method
hfus	44.31	kJ/mol	Joback Method
hvap	72.87	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.226		Crippen Method
mcvol	266.650	ml/mol	McGowan Method
pc	1483.85	kPa	Joback Method
rinpol	1883.00		NIST Webbook
rinpol	1883.00		NIST Webbook
tb	742.62	K	Joback Method
tc	928.32	K	Joback Method
tf	475.11	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	781.87	J/mol×K	742.62	Joback Method
cpg	798.44	J/mol×K	773.57	Joback Method
cpg	814.07	J/mol×K	804.52	Joback Method
cpg	828.81	J/mol×K	835.47	Joback Method
cpg	842.66	J/mol×K	866.42	Joback Method
cpg	855.65	J/mol×K	897.37	Joback Method
cpg	867.80	J/mol×K	928.32	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=U392375&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