DL-Alanine, N-methyl-N-(byt-3-yn-1-yloxycarbonyl)-, hexyl ester

Inchi: InChI=1S/C15H25NO4/c1-5-7-9-10-12-19-14(17)13(3)16(4)15(18)20-11-8-6-2/h2,13H,5,
InchiKey: JUFDEMFANLEZAH-UHFFFAOYSA-N
Formula: C15H25NO4
SMILES: C#CCCOC(=O)N(C)C(C)C(=O)OCCCCCC
Mol. weight [g/mol]: 283.36

Physical Properties

Property code	Value	Unit	Source
gf	-61.01	kJ/mol	Joback Method
hf	-488.38	kJ/mol	Joback Method
hfus	42.65	kJ/mol	Joback Method
hvap	68.81	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	2.590		Crippen Method
mcvol	238.470	ml/mol	McGowan Method
pc	1718.88	kPa	Joback Method
rinpol	1858.00		NIST Webbook
rinpol	1858.00		NIST Webbook
tb	697.30	K	Joback Method
tc	881.42	K	Joback Method
tf	467.57	K	Joback Method
vc	0.897	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	669.36	J/mol×K	697.30	Joback Method
cpg	684.96	J/mol×K	727.99	Joback Method
cpg	699.73	J/mol×K	758.67	Joback Method
cpg	713.70	J/mol×K	789.36	Joback Method
cpg	726.88	J/mol×K	820.05	Joback Method
cpg	739.28	J/mol×K	850.73	Joback Method
cpg	750.93	J/mol×K	881.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392703&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

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