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

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

InchiKey: SBZATZTVNCHNJI-UHFFFAOYSA-N

Formula: C17H29NO4

SMILES: C#CCCOC(=O)N(C)C(C)C(=O)OCCCCCCCC

Mol. weight [g/mol]: 311.42

Physical Properties

Property code	Value	Unit	Source
gf	-44.17	kJ/mol	Joback Method
hf	-529.66	kJ/mol	Joback Method
hfus	47.83	kJ/mol	Joback Method
hvap	73.26	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.370		Crippen Method
mcvol	266.650	ml/mol	McGowan Method
pc	1474.75	kPa	Joback Method
rinpol	2040.00		NIST Webbook
rinpol	2040.00		NIST Webbook
tb	743.06	K	Joback Method
tc	926.74	K	Joback Method
tf	490.11	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	781.37	J/mol×K	743.06	Joback Method
cpg	797.74	J/mol×K	773.67	Joback Method
cpg	813.21	J/mol×K	804.29	Joback Method
cpg	827.80	J/mol×K	834.90	Joback Method
cpg	841.54	J/mol×K	865.51	Joback Method
cpg	854.45	J/mol×K	896.13	Joback Method
cpg	866.54	J/mol×K	926.74	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=U392705&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