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

Inchi: InChI=1S/C13H21NO4/c1-5-7-9-17-12(15)11(3)14(4)13(16)18-10-8-6-2/h2,11H,5,7-10H2
InchiKey: OFZZXCRJBHLTOD-UHFFFAOYSA-N
Formula: C13H21NO4
SMILES: C#CCCOC(=O)N(C)C(C)C(=O)OCCCC
Mol. weight [g/mol]: 255.31

Physical Properties

Property code	Value	Unit	Source
gf	-77.85	kJ/mol	Joback Method
hf	-447.10	kJ/mol	Joback Method
hfus	37.47	kJ/mol	Joback Method
hvap	64.36	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	1.810		Crippen Method
mcvol	210.290	ml/mol	McGowan Method
pc	2029.06	kPa	Joback Method
rinpol	1664.00		NIST Webbook
rinpol	1664.00		NIST Webbook
tb	651.54	K	Joback Method
tc	837.93	K	Joback Method
tf	445.03	K	Joback Method
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	562.16	J/mol×K	651.54	Joback Method
cpg	576.84	J/mol×K	682.60	Joback Method
cpg	590.77	J/mol×K	713.67	Joback Method
cpg	603.95	J/mol×K	744.73	Joback Method
cpg	616.41	J/mol×K	775.80	Joback Method
cpg	628.16	J/mol×K	806.86	Joback Method
cpg	639.20	J/mol×K	837.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392701&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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