DL-Alanine, N-methyl-N-(byt-2-yn-1-yloxycarbonyl)-, but-2-yn-1-yl ester

Inchi: InChI=1S/C13H17NO4/c1-5-7-9-17-12(15)11(3)14(4)13(16)18-10-8-6-2/h11H,9-10H2,1-4

InchiKey: TXGBWXRPNIOLEI-UHFFFAOYSA-N

Formula: C13H17NO4

SMILES: CC#CCOC(=O)C(C)N(C)C(=O)OCC#CC

Mol. weight [g/mol]: 251.28

Physical Properties

Property code	Value	Unit	Source
gf	104.68	kJ/mol	Joback Method
hf	-194.40	kJ/mol	Joback Method
hfus	40.74	kJ/mol	Joback Method
hvap	68.80	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	1.033		Crippen Method
mcvol	201.690	ml/mol	McGowan Method
pc	2384.19	kPa	Joback Method
rinpol	1862.00		NIST Webbook
rinpol	1862.00		NIST Webbook
tb	679.42	K	Joback Method
tc	893.45	K	Joback Method
tf	610.26	K	Joback Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.20	J/mol×K	679.42	Joback Method
cpg	535.70	J/mol×K	715.09	Joback Method
cpg	549.35	J/mol×K	750.76	Joback Method
cpg	562.16	J/mol×K	786.43	Joback Method
cpg	574.13	J/mol×K	822.11	Joback Method
cpg	585.26	J/mol×K	857.78	Joback Method
cpg	595.56	J/mol×K	893.45	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=U392730&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