DL-Alanyl-DL-alanine, N,N'-dimethyl-N'-(byt-3-yn-1-yloxycarbonyl)-, byt-3-yn-1-yl ester

Inchi: InChI=1S/C17H24N2O5/c1-7-9-11-23-16(21)14(4)18(5)15(20)13(3)19(6)17(22)24-12-10-

InchiKey: PFGKWNHLVNEQGW-UHFFFAOYSA-N

Formula: C17H24N2O5

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

Mol. weight [g/mol]: 336.38

Physical Properties

Property code	Value	Unit	Source
gf	158.32	kJ/mol	Joback Method
hf	-288.09	kJ/mol	Joback Method
hfus	51.90	kJ/mol	Joback Method
hvap	81.52	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	0.880		Crippen Method
mcvol	269.600	ml/mol	McGowan Method
pc	1755.07	kPa	Joback Method
rinpol	2169.00		NIST Webbook
rinpol	2169.00		NIST Webbook
tb	799.05	K	Joback Method
tc	997.94	K	Joback Method
tf	604.48	K	Joback Method
vc	0.990	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	789.92	J/mol×K	799.05	Joback Method
cpg	804.13	J/mol×K	832.20	Joback Method
cpg	817.40	J/mol×K	865.35	Joback Method
cpg	829.74	J/mol×K	898.49	Joback Method
cpg	841.20	J/mol×K	931.64	Joback Method
cpg	851.82	J/mol×K	964.79	Joback Method
cpg	861.62	J/mol×K	997.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392714&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