DL-Valyl-DL-Valine, N,N'-dimethyl-N'-(but-3-yn-1-yloxycarbonyl)-, butyl ester

Inchi: InChI=1S/C21H36N2O5/c1-9-11-13-27-20(25)18(16(5)6)22(7)19(24)17(15(3)4)23(8)21(2

InchiKey: XMWLHYLAJDSWRH-UHFFFAOYSA-N

Formula: C21H36N2O5

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

Mol. weight [g/mol]: 396.52

Physical Properties

Property code	Value	Unit	Source
gf	-35.95	kJ/mol	Joback Method
hf	-673.11	kJ/mol	Joback Method
hfus	52.24	kJ/mol	Joback Method
hvap	89.79	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	2.929		Crippen Method
mcvol	334.560	ml/mol	McGowan Method
pc	1186.60	kPa	Joback Method
rinpol	2327.00		NIST Webbook
rinpol	2327.00		NIST Webbook
tb	899.57	K	Joback Method
tc	1103.24	K	Joback Method
tf	572.59	K	Joback Method
vc	1.240	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1082.30	J/mol×K	899.57	Joback Method
cpg	1098.71	J/mol×K	933.51	Joback Method
cpg	1113.89	J/mol×K	967.46	Joback Method
cpg	1127.88	J/mol×K	1001.40	Joback Method
cpg	1140.74	J/mol×K	1035.35	Joback Method
cpg	1152.50	J/mol×K	1069.29	Joback Method
cpg	1163.22	J/mol×K	1103.24	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=U392945&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