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

Inchi: InChI=1S/C21H32N2O5/c1-9-11-13-27-20(25)18(16(5)6)22(7)19(24)17(15(3)4)23(8)21(2

InchiKey: PRJFTFFBZUEASE-UHFFFAOYSA-N

Formula: C21H32N2O5

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

Mol. weight [g/mol]: 392.49

Physical Properties

Property code	Value	Unit	Source
gf	187.12	kJ/mol	Joback Method
hf	-381.21	kJ/mol	Joback Method
hfus	55.22	kJ/mol	Joback Method
hvap	89.65	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	2.152		Crippen Method
mcvol	325.960	ml/mol	McGowan Method
pc	1317.52	kPa	Joback Method
rinpol	2351.00		NIST Webbook
rinpol	2351.00		NIST Webbook
tb	889.69	K	Joback Method
tc	1095.05	K	Joback Method
tf	619.56	K	Joback Method
vc	1.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1023.68	J/mol×K	889.69	Joback Method
cpg	1039.18	J/mol×K	923.92	Joback Method
cpg	1053.54	J/mol×K	958.14	Joback Method
cpg	1066.83	J/mol×K	992.37	Joback Method
cpg	1079.08	J/mol×K	1026.60	Joback Method
cpg	1090.35	J/mol×K	1060.83	Joback Method
cpg	1100.69	J/mol×K	1095.05	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392951&Units=SI

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