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

Inchi: InChI=1S/C22H38N2O5/c1-9-11-13-15-28-21(26)19(17(5)6)23(7)20(25)18(16(3)4)24(8)2
InchiKey: LDKKTOFVKNJUBI-UHFFFAOYSA-N
Formula: C22H38N2O5
SMILES: C#CCCOC(=O)N(C)C(C(=O)N(C)C(C(=O)OCCCCC)C(C)C)C(C)C
Mol. weight [g/mol]: 410.55

Physical Properties

Property code	Value	Unit	Source
gf	-27.53	kJ/mol	Joback Method
hf	-693.75	kJ/mol	Joback Method
hfus	54.83	kJ/mol	Joback Method
hvap	92.02	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	3.319		Crippen Method
mcvol	348.650	ml/mol	McGowan Method
pc	1111.85	kPa	Joback Method
rinpol	2420.00		NIST Webbook
rinpol	2420.00		NIST Webbook
tb	922.45	K	Joback Method
tc	1129.82	K	Joback Method
tf	583.86	K	Joback Method
vc	1.296	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1143.27	J/mol×K	922.45	Joback Method
cpg	1159.96	J/mol×K	957.01	Joback Method
cpg	1175.35	J/mol×K	991.57	Joback Method
cpg	1189.51	J/mol×K	1026.14	Joback Method
cpg	1202.48	J/mol×K	1060.70	Joback Method
cpg	1214.31	J/mol×K	1095.26	Joback Method
cpg	1225.05	J/mol×K	1129.82	Joback Method

Sources

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=U392946&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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