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

Inchi: InChI=1S/C24H42N2O5/c1-9-11-13-14-15-17-30-23(28)21(19(5)6)25(7)22(27)20(18(3)4)
Inchikey: PLSTYUFEDIDQAL-UHFFFAOYSA-N
Formula: C24H42N2O5
SMILES: C#CCCOC(=O)N(C)C(C(=O)N(C)C(C(=O)OCCCCCCC)C(C)C)C(C)C
Mol. weight [g/mol]: 438.60

Physical Properties

Property code	Value	Unit	Source
gf	-10.69	kJ/mol	Joback Method
hf	-735.03	kJ/mol	Joback Method
hfus	60.01	kJ/mol	Joback Method
hvap	96.47	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	4.099		Crippen Method
mcvol	376.830	ml/mol	McGowan Method
pc	982.08	kPa	Joback Method
rinpol	2614.00		NIST Webbook
rinpol	2614.00		NIST Webbook
tb	968.21	K	Joback Method
tc	1185.89	K	Joback Method
tf	606.40	K	Joback Method
vc	1.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1266.83	J/mol×K	968.21	Joback Method
cpg	1284.16	J/mol×K	1004.49	Joback Method
cpg	1300.05	J/mol×K	1040.77	Joback Method
cpg	1314.56	J/mol×K	1077.05	Joback Method
cpg	1327.76	J/mol×K	1113.33	Joback Method
cpg	1339.71	J/mol×K	1149.61	Joback Method
cpg	1350.48	J/mol×K	1185.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392948&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