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

Inchi: InChI=1S/C23H40N2O5/c1-9-11-13-14-16-29-22(27)20(18(5)6)24(7)21(26)19(17(3)4)25(
InchiKey: YTQSTSRETRALLX-UHFFFAOYSA-N
Formula: C23H40N2O5
SMILES: C#CCCOC(=O)N(C)C(C(=O)N(C)C(C(=O)OCCCCCC)C(C)C)C(C)C
Mol. weight [g/mol]: 424.57

Physical Properties

Property code	Value	Unit	Source
gf	-19.11	kJ/mol	Joback Method
hf	-714.39	kJ/mol	Joback Method
hfus	57.42	kJ/mol	Joback Method
hvap	94.24	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	3.709		Crippen Method
mcvol	362.740	ml/mol	McGowan Method
pc	1043.95	kPa	Joback Method
rinpol	2518.00		NIST Webbook
rinpol	2518.00		NIST Webbook
tb	945.33	K	Joback Method
tc	1157.35	K	Joback Method
tf	595.13	K	Joback Method
vc	1.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1204.80	J/mol×K	945.33	Joback Method
cpg	1221.79	J/mol×K	980.67	Joback Method
cpg	1237.42	J/mol×K	1016.00	Joback Method
cpg	1251.75	J/mol×K	1051.34	Joback Method
cpg	1264.83	J/mol×K	1086.68	Joback Method
cpg	1276.72	J/mol×K	1122.01	Joback Method
cpg	1287.48	J/mol×K	1157.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392947&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

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