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

Inchi: InChI=1S/C25H44N2O5/c1-9-11-13-14-15-16-18-31-24(29)22(20(5)6)26(7)23(28)21(19(3

InchiKey: LYILOXSDVVJYCH-UHFFFAOYSA-N

Formula: C25H44N2O5

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

Mol. weight [g/mol]: 452.63

Physical Properties

Property code	Value	Unit	Source
gf	-2.27	kJ/mol	Joback Method
hf	-755.67	kJ/mol	Joback Method
hfus	62.60	kJ/mol	Joback Method
hvap	98.69	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	4.489		Crippen Method
mcvol	390.920	ml/mol	McGowan Method
pc	925.55	kPa	Joback Method
rinpol	2721.00		NIST Webbook
rinpol	2721.00		NIST Webbook
tb	991.09	K	Joback Method
tc	1215.52	K	Joback Method
tf	617.67	K	Joback Method
vc	1.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1329.33	J/mol×K	991.09	Joback Method
cpg	1347.03	J/mol×K	1028.50	Joback Method
cpg	1363.20	J/mol×K	1065.90	Joback Method
cpg	1377.90	J/mol×K	1103.31	Joback Method
cpg	1391.22	J/mol×K	1140.71	Joback Method
cpg	1403.23	J/mol×K	1178.12	Joback Method
cpg	1414.01	J/mol×K	1215.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392949&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