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

Inchi: InChI=1S/C26H46N2O5/c1-9-11-13-14-15-16-17-19-32-25(30)23(21(5)6)27(7)24(29)22(2

InchiKey: GYLGSYJXCPDZKV-UHFFFAOYSA-N

Formula: C26H46N2O5

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

Mol. weight [g/mol]: 466.65

Physical Properties

Property code	Value	Unit	Source
gf	6.15	kJ/mol	Joback Method
hf	-776.31	kJ/mol	Joback Method
hfus	65.19	kJ/mol	Joback Method
hvap	100.92	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	4.880		Crippen Method
mcvol	405.010	ml/mol	McGowan Method
pc	873.77	kPa	Joback Method
rinpol	2823.00		NIST Webbook
rinpol	2823.00		NIST Webbook
tb	1013.97	K	Joback Method
tc	1246.32	K	Joback Method
tf	628.94	K	Joback Method
vc	1.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1392.24	J/mol×K	1013.97	Joback Method
cpg	1410.36	J/mol×K	1052.70	Joback Method
cpg	1426.83	J/mol×K	1091.42	Joback Method
cpg	1441.75	J/mol×K	1130.15	Joback Method
cpg	1455.20	J/mol×K	1168.87	Joback Method
cpg	1467.27	J/mol×K	1207.60	Joback Method
cpg	1478.04	J/mol×K	1246.32	Joback Method

Sources

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=U392950&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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