DL-Valine, N-methyl-N-(but-3-yn-1-yloxycarbonyl)-, pentadecyl ester

Inchi: InChI=1S/C26H47NO4/c1-6-8-10-11-12-13-14-15-16-17-18-19-20-22-30-25(28)24(23(3)4
InchiKey: FZWCZCSEIHCESL-UHFFFAOYSA-N
Formula: C26H47NO4
SMILES: C#CCCOC(=O)N(C)C(C(=O)OCCCCCCCCCCCCCCC)C(C)C
Mol. weight [g/mol]: 437.66

Physical Properties

Property code	Value	Unit	Source
gf	29.17	kJ/mol	Joback Method
hf	-720.70	kJ/mol	Joback Method
hfus	67.62	kJ/mol	Joback Method
hvap	92.91	kJ/mol	Joback Method
log10ws	-7.64		Crippen Method
logp	6.737		Crippen Method
mcvol	393.460	ml/mol	McGowan Method
pc	835.31	kPa	Joback Method
rinpol	2854.00		NIST Webbook
rinpol	2854.00		NIST Webbook
tb	948.54	K	Joback Method
tc	1163.59	K	Joback Method
tf	576.54	K	Joback Method
vc	1.508	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1329.01	J/mol×K	948.54	Joback Method
cpg	1348.94	J/mol×K	984.38	Joback Method
cpg	1367.38	J/mol×K	1020.22	Joback Method
cpg	1384.39	J/mol×K	1056.07	Joback Method
cpg	1400.03	J/mol×K	1091.91	Joback Method
cpg	1414.36	J/mol×K	1127.75	Joback Method
cpg	1427.45	J/mol×K	1163.59	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392941&Units=SI

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