DL-Valine, N-methyl-N-(but-2-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: HOTXVBFHEXJUNH-UHFFFAOYSA-N
Formula: C26H47NO4
SMILES: CC#CCOC(=O)N(C)C(C(=O)OCCCCCCCCCCCCCCC)C(C)C
Mol. weight [g/mol]: 437.66

Physical Properties

Property code	Value	Unit	Source
gf	8.90	kJ/mol	Joback Method
hf	-740.30	kJ/mol	Joback Method
hfus	67.77	kJ/mol	Joback Method
hvap	95.20	kJ/mol	Joback Method
log10ws	-7.64		Crippen Method
logp	6.737		Crippen Method
mcvol	393.460	ml/mol	McGowan Method
pc	841.13	kPa	Joback Method
rinpol	2937.00		NIST Webbook
rinpol	2937.00		NIST Webbook
tb	967.42	K	Joback Method
tc	1186.15	K	Joback Method
tf	635.67	K	Joback Method
vc	1.508	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1336.16	J/mol×K	967.42	Joback Method
cpg	1355.72	J/mol×K	1003.88	Joback Method
cpg	1373.68	J/mol×K	1040.33	Joback Method
cpg	1390.11	J/mol×K	1076.79	Joback Method
cpg	1405.06	J/mol×K	1113.24	Joback Method
cpg	1418.57	J/mol×K	1149.70	Joback Method
cpg	1430.72	J/mol×K	1186.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392960&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