DL-Valine, N-methyl-N-(but-2-yn-1-yloxycarbonyl)-, decyl ester

Inchi: InChI=1S/C21H37NO4/c1-6-8-10-11-12-13-14-15-17-25-20(23)19(18(3)4)22(5)21(24)26-
InchiKey: GFQPBIDQJSVXFD-UHFFFAOYSA-N
Formula: C21H37NO4
SMILES: CC#CCOC(=O)N(C)C(C(=O)OCCCCCCCCCC)C(C)C
Mol. weight [g/mol]: 367.52

Physical Properties

Property code	Value	Unit	Source
gf	-33.20	kJ/mol	Joback Method
hf	-637.10	kJ/mol	Joback Method
hfus	54.82	kJ/mol	Joback Method
hvap	84.07	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	4.787		Crippen Method
mcvol	323.010	ml/mol	McGowan Method
pc	1135.20	kPa	Joback Method
rinpol	2437.00		NIST Webbook
rinpol	2437.00		NIST Webbook
tb	853.02	K	Joback Method
tc	1048.91	K	Joback Method
tf	579.32	K	Joback Method
vc	1.228	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1024.22	J/mol×K	853.02	Joback Method
cpg	1042.13	J/mol×K	885.67	Joback Method
cpg	1058.86	J/mol×K	918.32	Joback Method
cpg	1074.45	J/mol×K	950.97	Joback Method
cpg	1088.91	J/mol×K	983.62	Joback Method
cpg	1102.29	J/mol×K	1016.26	Joback Method
cpg	1114.59	J/mol×K	1048.91	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=U392955&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