DL-Valine, N-methyl-N-(but-3-en-1-yloxycarbonyl)-, decyl ester

Inchi: InChI=1S/C21H39NO4/c1-6-8-10-11-12-13-14-15-17-25-20(23)19(18(3)4)22(5)21(24)26-

InchiKey: PNIZDWDVLICXIU-UHFFFAOYSA-N

Formula: C21H39NO4

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

Mol. weight [g/mol]: 369.54

Physical Properties

Property code	Value	Unit	Source
gf	-148.16	kJ/mol	Joback Method
hf	-783.97	kJ/mol	Joback Method
hfus	50.41	kJ/mol	Joback Method
hvap	81.25	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	5.339		Crippen Method
mcvol	327.310	ml/mol	McGowan Method
pc	1050.05	kPa	Joback Method
rinpol	2361.00		NIST Webbook
rinpol	2361.00		NIST Webbook
tb	840.70	K	Joback Method
tc	1030.77	K	Joback Method
tf	471.46	K	Joback Method
vc	1.246	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1047.23	J/mol×K	840.70	Joback Method
cpg	1065.61	J/mol×K	872.38	Joback Method
cpg	1082.84	J/mol×K	904.06	Joback Method
cpg	1098.96	J/mol×K	935.74	Joback Method
cpg	1114.00	J/mol×K	967.41	Joback Method
cpg	1127.99	J/mol×K	999.09	Joback Method
cpg	1140.96	J/mol×K	1030.77	Joback Method

Sources

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=U392962&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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