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

Inchi: InChI=1S/C22H41NO4/c1-6-8-10-11-12-13-14-15-16-18-26-21(24)20(19(3)4)23(5)22(25)
InchiKey: DVWQOCNCZSSWGP-UHFFFAOYSA-N
Formula: C22H41NO4
SMILES: C=CCCOC(=O)N(C)C(C(=O)OCCCCCCCCCCC)C(C)C
Mol. weight [g/mol]: 383.57

Physical Properties

Property code	Value	Unit	Source
gf	-139.74	kJ/mol	Joback Method
hf	-804.61	kJ/mol	Joback Method
hfus	53.01	kJ/mol	Joback Method
hvap	83.47	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	5.730		Crippen Method
mcvol	341.400	ml/mol	McGowan Method
pc	987.64	kPa	Joback Method
rinpol	2459.00		NIST Webbook
rinpol	2459.00		NIST Webbook
tb	863.58	K	Joback Method
tc	1057.59	K	Joback Method
tf	482.73	K	Joback Method
vc	1.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1108.85	J/mol×K	863.58	Joback Method
cpg	1127.61	J/mol×K	895.91	Joback Method
cpg	1145.17	J/mol×K	928.25	Joback Method
cpg	1161.54	J/mol×K	960.58	Joback Method
cpg	1176.77	J/mol×K	992.92	Joback Method
cpg	1190.90	J/mol×K	1025.25	Joback Method
cpg	1203.96	J/mol×K	1057.59	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=U392963&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