DL-Valine, N-methyl-N-(vinyloxycarbonyl)-, tetradecyl ester

Inchi: InChI=1S/C23H43NO4/c1-6-8-9-10-11-12-13-14-15-16-17-18-19-28-22(25)21(20(3)4)24(
InchiKey: TXLLBCKYNVUNKP-UHFFFAOYSA-N
Formula: C23H43NO4
SMILES: C=COC(=O)N(C)C(C(=O)OCCCCCCCCCCCCCC)C(C)C
Mol. weight [g/mol]: 397.59

Physical Properties

Property code	Value	Unit	Source
gf	-131.32	kJ/mol	Joback Method
hf	-825.25	kJ/mol	Joback Method
hfus	55.60	kJ/mol	Joback Method
hvap	85.70	kJ/mol	Joback Method
log10ws	-6.94		Crippen Method
logp	6.467		Crippen Method
mcvol	355.490	ml/mol	McGowan Method
pc	930.64	kPa	Joback Method
rinpol	2564.00		NIST Webbook
rinpol	2564.00		NIST Webbook
tb	886.46	K	Joback Method
tc	1085.29	K	Joback Method
tf	494.00	K	Joback Method
vc	1.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1171.10	J/mol×K	886.46	Joback Method
cpg	1190.29	J/mol×K	919.60	Joback Method
cpg	1208.19	J/mol×K	952.74	Joback Method
cpg	1224.83	J/mol×K	985.87	Joback Method
cpg	1240.26	J/mol×K	1019.01	Joback Method
cpg	1254.52	J/mol×K	1052.15	Joback Method
cpg	1267.65	J/mol×K	1085.29	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=U393045&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