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

Inchi: InChI=1S/C19H35NO4/c1-6-8-9-10-11-12-13-14-15-24-18(21)17(16(3)4)20(5)19(22)23-7

InchiKey: GJGYDJTYCGURKK-UHFFFAOYSA-N

Formula: C19H35NO4

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

Mol. weight [g/mol]: 341.49

Physical Properties

Property code	Value	Unit	Source
gf	-165.00	kJ/mol	Joback Method
hf	-742.69	kJ/mol	Joback Method
hfus	45.23	kJ/mol	Joback Method
hvap	76.80	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	4.907		Crippen Method
mcvol	299.130	ml/mol	McGowan Method
pc	1194.00	kPa	Joback Method
rinpol	2133.00		NIST Webbook
rinpol	2133.00		NIST Webbook
tb	794.94	K	Joback Method
tc	979.53	K	Joback Method
tf	448.92	K	Joback Method
vc	1.135	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	926.19	J/mol×K	794.94	Joback Method
cpg	943.84	J/mol×K	825.71	Joback Method
cpg	960.47	J/mol×K	856.47	Joback Method
cpg	976.10	J/mol×K	887.24	Joback Method
cpg	990.74	J/mol×K	918.00	Joback Method
cpg	1004.44	J/mol×K	948.77	Joback Method
cpg	1017.20	J/mol×K	979.53	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=U393041&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