DL-Valine, N-methyl-N-(2-ethylhexyloxycarbonyl)-, octadecyl ester

Inchi: InChI=1S/C33H65NO4/c1-7-10-12-13-14-15-16-17-18-19-20-21-22-23-24-25-27-37-32(3
InchiKey: DCIIXTLFVRMOOG-UHFFFAOYSA-N
Formula: C33H65NO4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(C(C)C)N(C)C(=O)OCC(CC)CCCC
Mol. weight [g/mol]: 539.87

Physical Properties

Property code	Value	Unit	Source
gf	-137.40	kJ/mol	Joback Method
hf	-1162.36	kJ/mol	Joback Method
hfus	79.25	kJ/mol	Joback Method
hvap	108.24	kJ/mol	Joback Method
log10ws	-10.54		Crippen Method
logp	10.101		Crippen Method
mcvol	500.690	ml/mol	McGowan Method
pc	547.95	kPa	Joback Method
rinpol	3436.00		NIST Webbook
rinpol	3436.00		NIST Webbook
tb	1118.14	K	Joback Method
tc	1434.75	K	Joback Method
tf	593.46	K	Joback Method
vc	1.931	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1848.88	J/mol×K	1118.14	Joback Method
cpg	1875.06	J/mol×K	1170.91	Joback Method
cpg	1897.80	J/mol×K	1223.68	Joback Method
cpg	1917.37	J/mol×K	1276.45	Joback Method
cpg	1934.01	J/mol×K	1329.22	Joback Method
cpg	1947.99	J/mol×K	1381.98	Joback Method
cpg	1959.56	J/mol×K	1434.75	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392922&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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