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

Inchi: InChI=1S/C31H61NO4/c1-7-10-12-13-14-15-16-17-18-19-20-21-22-23-25-35-30(33)29(2
InchiKey: ZGGCIZJXPXGHIH-UHFFFAOYSA-N
Formula: C31H61NO4
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(C(C)C)N(C)C(=O)OCC(CC)CCCC
Mol. weight [g/mol]: 511.82

Physical Properties

Property code	Value	Unit	Source
gf	-154.24	kJ/mol	Joback Method
hf	-1121.08	kJ/mol	Joback Method
hfus	74.07	kJ/mol	Joback Method
hvap	103.79	kJ/mol	Joback Method
log10ws	-9.70		Crippen Method
logp	9.320		Crippen Method
mcvol	472.510	ml/mol	McGowan Method
pc	600.73	kPa	Joback Method
rinpol	3230.00		NIST Webbook
rinpol	3230.00		NIST Webbook
tb	1072.38	K	Joback Method
tc	1353.11	K	Joback Method
tf	570.92	K	Joback Method
vc	1.819	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1717.03	J/mol×K	1072.38	Joback Method
cpg	1741.51	J/mol×K	1119.17	Joback Method
cpg	1763.22	J/mol×K	1165.96	Joback Method
cpg	1782.32	J/mol×K	1212.74	Joback Method
cpg	1798.98	J/mol×K	1259.53	Joback Method
cpg	1813.36	J/mol×K	1306.32	Joback Method
cpg	1825.63	J/mol×K	1353.11	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=U392920&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