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

Inchi: InChI=1S/C32H63NO4/c1-7-10-12-13-14-15-16-17-18-19-20-21-22-23-24-26-36-31(34)3
InchiKey: GWGXOWNBIKSINP-UHFFFAOYSA-N
Formula: C32H63NO4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(C(C)C)N(C)C(=O)OCC(CC)CCCC
Mol. weight [g/mol]: 525.85

Physical Properties

Property code	Value	Unit	Source
gf	-145.82	kJ/mol	Joback Method
hf	-1141.72	kJ/mol	Joback Method
hfus	76.66	kJ/mol	Joback Method
hvap	106.02	kJ/mol	Joback Method
log10ws	-10.12		Crippen Method
logp	9.710		Crippen Method
mcvol	486.600	ml/mol	McGowan Method
pc	573.43	kPa	Joback Method
rinpol	3332.00		NIST Webbook
rinpol	3332.00		NIST Webbook
tb	1095.26	K	Joback Method
tc	1392.95	K	Joback Method
tf	582.19	K	Joback Method
vc	1.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1782.88	J/mol×K	1095.26	Joback Method
cpg	1808.18	J/mol×K	1144.88	Joback Method
cpg	1830.40	J/mol×K	1194.49	Joback Method
cpg	1849.74	J/mol×K	1244.11	Joback Method
cpg	1866.42	J/mol×K	1293.72	Joback Method
cpg	1880.62	J/mol×K	1343.34	Joback Method
cpg	1892.56	J/mol×K	1392.95	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U392921&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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