L-Leucine, N-methyl-N-(hexyloxycarbonyl)-, eicosyl ester

Inchi: InChI=1S/C34H67NO4/c1-6-8-10-12-13-14-15-16-17-18-19-20-21-22-23-24-25-27-28-38

InchiKey: NPWFJRXQVYSMDY-JGCGQSQUSA-N

Formula: C34H67NO4

SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCCCCCC

Mol. weight [g/mol]: 553.90

Physical Properties

Property code	Value	Unit	Source
gf	-126.54	kJ/mol	Joback Method
hf	-1177.72	kJ/mol	Joback Method
hfus	85.37	kJ/mol	Joback Method
hvap	110.86	kJ/mol	Joback Method
log10ws	-11.20		Crippen Method
logp	10.635		Crippen Method
mcvol	514.780	ml/mol	McGowan Method
pc	522.21	kPa	Joback Method
rinpol	3500.00		NIST Webbook
rinpol	3500.00		NIST Webbook
tb	1141.46	K	Joback Method
tc	1485.32	K	Joback Method
tf	619.73	K	Joback Method
vc	1.994	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1915.07	J/mol×K	1141.46	Joback Method
cpg	1942.82	J/mol×K	1198.77	Joback Method
cpg	1966.64	J/mol×K	1256.08	Joback Method
cpg	1986.86	J/mol×K	1313.39	Joback Method
cpg	2003.83	J/mol×K	1370.70	Joback Method
cpg	2017.89	J/mol×K	1428.01	Joback Method
cpg	2029.38	J/mol×K	1485.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392357&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