L-Leucine, N-methyl-N-((1R)-(-)-menthyloxycarbonyl)-, tetradecyl ester

Inchi: InChI=1S/C32H61NO4/c1-8-9-10-11-12-13-14-15-16-17-18-19-22-36-31(34)29(23-25(2)3
InchiKey: IXVISAGXVHUNHJ-UHFFFAOYSA-N
Formula: C32H61NO4
SMILES: CCCCCCCCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OC1CC(C)CCC1C(C)C
Mol. weight [g/mol]: 523.83

Physical Properties

Property code	Value	Unit	Source
gf	-136.79	kJ/mol	Joback Method
hf	-1128.08	kJ/mol	Joback Method
hfus	70.64	kJ/mol	Joback Method
hvap	105.83	kJ/mol	Joback Method
log10ws	-9.64		Crippen Method
logp	9.175		Crippen Method
mcvol	475.740	ml/mol	McGowan Method
pc	613.60	kPa	Joback Method
rinpol	3267.00		NIST Webbook
rinpol	3267.00		NIST Webbook
tb	1105.47	K	Joback Method
tc	1378.99	K	Joback Method
tf	581.09	K	Joback Method
vc	1.806	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1784.22	J/mol×K	1105.47	Joback Method
cpg	1805.05	J/mol×K	1151.06	Joback Method
cpg	1822.76	J/mol×K	1196.64	Joback Method
cpg	1837.47	J/mol×K	1242.23	Joback Method
cpg	1849.32	J/mol×K	1287.82	Joback Method
cpg	1858.43	J/mol×K	1333.40	Joback Method
cpg	1864.95	J/mol×K	1378.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392421&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