

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

InChI: InChI=1S/C33H63NO4/c1-8-9-10-11-12-13-14-15-16-17-18-19-20-23-37-32(35)30(24-26)1
InChIKey: LXAXKDHNNFBUEN-UHFFFAOYSA-N

Formula: C33H63NO4

SMILES: CCCCCCCCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OC1CC(C)CCC1C(C)C

Mol. weight [g/mol]: 537.86

Physical Properties

Property code	Value	Unit	Source
gf	-128.37	kJ/mol	Joback Method
hf	-1148.72	kJ/mol	Joback Method
hfus	73.23	kJ/mol	Joback Method
hvap	108.05	kJ/mol	Joback Method
log10ws	-10.06		Crippen Method
logp	9.565		Crippen Method
mcvol	489.830	ml/mol	McGowan Method
pc	585.42	kPa	Joback Method
rinpol	3366.00		NIST Webbook
rinpol	3366.00		NIST Webbook
tb	1128.35	K	Joback Method
tc	1416.38	K	Joback Method
tf	592.36	K	Joback Method
vc	1.863	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1849.20	J/molxK	1128.35	Joback Method
cpg	1870.20	J/molxK	1176.36	Joback Method
cpg	1887.75	J/molxK	1224.36	Joback Method
cpg	1902.03	J/molxK	1272.37	Joback Method
cpg	1913.18	J/molxK	1320.37	Joback Method
cpg	1921.37	J/molxK	1368.38	Joback Method
cpg	1926.77	J/molxK	1416.38	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U392422&Units=SI

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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