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

Inchi: InChI=1S/C31H59NO4/c1-8-9-10-11-12-13-14-15-16-17-18-21-35-30(33)28(22-24(2)3)32

InchiKey: IEACPNHLZRUODK-UHFFFAOYSA-N

Formula: C31H59NO4

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

Mol. weight [g/mol]: 509.80

Physical Properties

Property code	Value	Unit	Source
gf	-145.21	kJ/mol	Joback Method
hf	-1107.44	kJ/mol	Joback Method
hfus	68.05	kJ/mol	Joback Method
hvap	103.60	kJ/mol	Joback Method
log10ws	-9.22		Crippen Method
logp	8.784		Crippen Method
mcvol	461.650	ml/mol	McGowan Method
pc	643.85	kPa	Joback Method
rinpol	3168.00		NIST Webbook
rinpol	3168.00		NIST Webbook
tb	1082.59	K	Joback Method
tc	1343.25	K	Joback Method
tf	569.82	K	Joback Method
vc	1.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1719.27	J/mol×K	1082.59	Joback Method
cpg	1739.94	J/mol×K	1126.03	Joback Method
cpg	1757.75	J/mol×K	1169.48	Joback Method
cpg	1772.83	J/mol×K	1212.92	Joback Method
cpg	1785.27	J/mol×K	1256.36	Joback Method
cpg	1795.18	J/mol×K	1299.81	Joback Method
cpg	1802.67	J/mol×K	1343.25	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392420&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume