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

Inchi: InChI=1S/C30H57NO4/c1-8-9-10-11-12-13-14-15-16-17-20-34-29(32)27(21-23(2)3)31(7)30(33)35-26-22-24(4)18-19-25(26)28(5)6

InchiKey: IQBJWNPFEQEHBR-UHFFFAOYSA-N

Formula: C30H57NO4

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

Mol. weight [g/mol]: 495.78

Physical Properties

Property code	Value	Unit	Source
gf	-153.63	kJ/mol	Joback Method
hf	-1086.80	kJ/mol	Joback Method
hfus	65.46	kJ/mol	Joback Method
hvap	101.38	kJ/mol	Joback Method
log10ws	-8.80		Crippen Method
logp	8.394		Crippen Method
mcvol	447.560	ml/mol	McGowan Method
pc	676.41	kPa	Joback Method
rinpol	3070.00		NIST Webbook
rinpol	3070.00		NIST Webbook
tb	1059.71	K	Joback Method
tc	1309.04	K	Joback Method
tf	558.55	K	Joback Method
vc	1.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1654.36	J/mol×K	1059.71	Joback Method
cpg	1674.88	J/mol×K	1101.27	Joback Method
cpg	1692.78	J/mol×K	1142.82	Joback Method
cpg	1708.16	J/mol×K	1184.38	Joback Method
cpg	1721.10	J/mol×K	1225.93	Joback Method
cpg	1731.70	J/mol×K	1267.49	Joback Method
cpg	1740.05	J/mol×K	1309.04	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=U392419&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

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