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

Inchi: InChI=1S/C25H47NO4/c1-8-9-10-11-12-15-29-24(27)22(16-18(2)3)26(7)25(28)30-23-17-19(4)13-14-21(23)20(5)6

Inchikey: TYRJFPJQUXAKGB-UHFFFAOYSA-N

Formula: C25H47NO4

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

Mol. weight [g/mol]: 425.64

Physical Properties

Property code	Value	Unit	Source
gf	-195.73	kJ/mol	Joback Method
hf	-983.60	kJ/mol	Joback Method
hfus	52.51	kJ/mol	Joback Method
hvap	90.25	kJ/mol	Joback Method
log10ws	-6.71		Crippen Method
logp	6.444		Crippen Method
mcvol	377.110	ml/mol	McGowan Method
pc	883.14	kPa	Joback Method
rinpol	2563.00		NIST Webbook
rinpol	2563.00		NIST Webbook
tb	945.31	K	Joback Method
tc	1157.44	K	Joback Method
tf	502.20	K	Joback Method
vc	1.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1331.98	J/mol×K	945.31	Joback Method
cpg	1352.01	J/mol×K	980.67	Joback Method
cpg	1370.19	J/mol×K	1016.02	Joback Method
cpg	1386.59	J/mol×K	1051.38	Joback Method
cpg	1401.22	J/mol×K	1086.73	Joback Method
cpg	1414.13	J/mol×K	1122.09	Joback Method
cpg	1425.37	J/mol×K	1157.44	Joback Method

Sources

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=U392414&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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