L-Leucine, N-methyl-N-(2-ethylhexyloxycarbonyl)-, octyl ester

Inchi: InChI=1S/C24H47NO4/c1-7-10-12-13-14-15-17-28-23(26)22(18-20(4)5)25(6)24(27)29-19
InchiKey: NWPIDUAZYHOYFC-UHFFFAOYSA-N
Formula: C24H47NO4
SMILES: CCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCC(CC)CCCC
Mol. weight [g/mol]: 413.63

Physical Properties

Property code	Value	Unit	Source
gf	-213.18	kJ/mol	Joback Method
hf	-976.60	kJ/mol	Joback Method
hfus	55.94	kJ/mol	Joback Method
hvap	88.21	kJ/mol	Joback Method
log10ws	-6.77		Crippen Method
logp	6.590		Crippen Method
mcvol	373.880	ml/mol	McGowan Method
pc	861.00	kPa	Joback Method
rinpol	2427.00		NIST Webbook
rinpol	2427.00		NIST Webbook
tb	912.22	K	Joback Method
tc	1117.57	K	Joback Method
tf	492.03	K	Joback Method
vc	1.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1263.43	J/mol×K	912.22	Joback Method
cpg	1283.58	J/mol×K	946.44	Joback Method
cpg	1302.27	J/mol×K	980.67	Joback Method
cpg	1319.53	J/mol×K	1014.89	Joback Method
cpg	1335.42	J/mol×K	1049.12	Joback Method
cpg	1349.97	J/mol×K	1083.34	Joback Method
cpg	1363.24	J/mol×K	1117.57	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392391&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