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

Inchi: InChI=1S/C20H39NO4/c1-7-10-12-17(9-3)15-25-20(23)21(6)18(14-16(4)5)19(22)24-13-1
InchiKey: FDVFVRGTFZPJFU-UHFFFAOYSA-N
Formula: C20H39NO4
SMILES: CCCCOC(=O)C(CC(C)C)N(C)C(=O)OCC(CC)CCCC
Mol. weight [g/mol]: 357.53

Physical Properties

Property code	Value	Unit	Source
gf	-246.86	kJ/mol	Joback Method
hf	-894.04	kJ/mol	Joback Method
hfus	45.58	kJ/mol	Joback Method
hvap	79.30	kJ/mol	Joback Method
log10ws	-5.10		Crippen Method
logp	5.029		Crippen Method
mcvol	317.520	ml/mol	McGowan Method
pc	1093.54	kPa	Joback Method
rinpol	2076.00		NIST Webbook
rinpol	2076.00		NIST Webbook
tb	820.70	K	Joback Method
tc	1008.12	K	Joback Method
tf	446.95	K	Joback Method
vc	1.204	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1014.01	J/mol×K	820.70	Joback Method
cpg	1032.62	J/mol×K	851.94	Joback Method
cpg	1050.10	J/mol×K	883.17	Joback Method
cpg	1066.47	J/mol×K	914.41	Joback Method
cpg	1081.75	J/mol×K	945.64	Joback Method
cpg	1095.97	J/mol×K	976.88	Joback Method
cpg	1109.16	J/mol×K	1008.12	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=U392389&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