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

Inchi: InChI=1S/C22H43NO4/c1-8-10-13-19(9-2)16-27-22(25)23(7)20(15-18(5)6)21(24)26-14-1
InchiKey: PYKQTWCLZSKDRM-UHFFFAOYSA-N
Formula: C22H43NO4
SMILES: CCCCC(CC)COC(=O)N(C)C(CC(C)C)C(=O)OCCCC(C)C
Mol. weight [g/mol]: 385.58

Physical Properties

Property code	Value	Unit	Source
gf	-232.46	kJ/mol	Joback Method
hf	-940.60	kJ/mol	Joback Method
hfus	47.24	kJ/mol	Joback Method
hvap	83.37	kJ/mol	Joback Method
log10ws	-5.69		Crippen Method
logp	5.665		Crippen Method
mcvol	345.700	ml/mol	McGowan Method
pc	971.70	kPa	Joback Method
rinpol	2212.00		NIST Webbook
rinpol	2212.00		NIST Webbook
tb	866.02	K	Joback Method
tc	1060.86	K	Joback Method
tf	454.49	K	Joback Method
vc	1.310	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1137.95	J/mol×K	866.02	Joback Method
cpg	1157.28	J/mol×K	898.49	Joback Method
cpg	1175.33	J/mol×K	930.97	Joback Method
cpg	1192.12	J/mol×K	963.44	Joback Method
cpg	1207.68	J/mol×K	995.91	Joback Method
cpg	1222.04	J/mol×K	1028.38	Joback Method
cpg	1235.25	J/mol×K	1060.86	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=U392399&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