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

Inchi: InChI=1S/C20H39NO4/c1-8-10-11-17(9-2)14-25-20(23)21(7)18(12-15(3)4)19(22)24-13-1
InchiKey: UDMFZLUNHJAAKK-UHFFFAOYSA-N
Formula: C20H39NO4
SMILES: CCCCC(CC)COC(=O)N(C)C(CC(C)C)C(=O)OCC(C)C
Mol. weight [g/mol]: 357.53

Physical Properties

Property code	Value	Unit	Source
gf	-249.30	kJ/mol	Joback Method
hf	-899.32	kJ/mol	Joback Method
hfus	42.06	kJ/mol	Joback Method
hvap	78.92	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	4.885		Crippen Method
mcvol	317.520	ml/mol	McGowan Method
pc	1099.35	kPa	Joback Method
rinpol	2037.00		NIST Webbook
rinpol	2037.00		NIST Webbook
tb	820.26	K	Joback Method
tc	1008.59	K	Joback Method
tf	431.95	K	Joback Method
vc	1.198	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1014.48	J/mol×K	820.26	Joback Method
cpg	1033.19	J/mol×K	851.65	Joback Method
cpg	1050.73	J/mol×K	883.04	Joback Method
cpg	1067.15	J/mol×K	914.42	Joback Method
cpg	1082.46	J/mol×K	945.81	Joback Method
cpg	1096.69	J/mol×K	977.20	Joback Method
cpg	1109.87	J/mol×K	1008.59	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=U392398&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