l-Leucine, N-ethoxycarbonyl-N-methyl-, isobutyl ester

Inchi: InChI=1S/C14H27NO4/c1-7-18-14(17)15(6)12(8-10(2)3)13(16)19-9-11(4)5/h10-12H,7-9H

InchiKey: IEBCWZJJTRIGJR-UHFFFAOYSA-N

Formula: C14H27NO4

SMILES: CCOC(=O)N(C)C(CC(C)C)C(=O)OCC(C)C

Mol. weight [g/mol]: 273.37

Physical Properties

Property code	Value	Unit	Source
gf	-297.38	kJ/mol	Joback Method
hf	-770.20	kJ/mol	Joback Method
hfus	30.04	kJ/mol	Joback Method
hvap	65.95	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.689		Crippen Method
mcvol	232.980	ml/mol	McGowan Method
pc	1668.70	kPa	Joback Method
rinpol	1614.00		NIST Webbook
tb	683.42	K	Joback Method
tc	865.73	K	Joback Method
tf	379.33	K	Joback Method
vc	0.868	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	663.68	J/mol×K	683.42	Joback Method
cpg	680.30	J/mol×K	713.80	Joback Method
cpg	696.07	J/mol×K	744.19	Joback Method
cpg	710.99	J/mol×K	774.57	Joback Method
cpg	725.07	J/mol×K	804.96	Joback Method
cpg	738.33	J/mol×K	835.34	Joback Method
cpg	750.77	J/mol×K	865.73	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=U321921&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