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

Inchi: InChI=1S/C16H31NO4/c1-11(2)8-14(15(18)20-9-12(3)4)17(7)16(19)21-10-13(5)6/h11-14

InchiKey: JOMTYNZJCKLJBL-UHFFFAOYSA-N

Formula: C16H31NO4

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

Mol. weight [g/mol]: 301.42

Physical Properties

Property code	Value	Unit	Source
gf	-282.98	kJ/mol	Joback Method
hf	-816.76	kJ/mol	Joback Method
hfus	31.70	kJ/mol	Joback Method
hvap	70.01	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	3.325		Crippen Method
mcvol	261.160	ml/mol	McGowan Method
pc	1443.54	kPa	Joback Method
rinpol	1760.00		NIST Webbook
rinpol	1760.00		NIST Webbook
tb	728.74	K	Joback Method
tc	912.54	K	Joback Method
tf	386.87	K	Joback Method
vc	0.974	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	776.97	J/mol×K	728.74	Joback Method
cpg	794.52	J/mol×K	759.37	Joback Method
cpg	811.11	J/mol×K	790.01	Joback Method
cpg	826.75	J/mol×K	820.64	Joback Method
cpg	841.45	J/mol×K	851.28	Joback Method
cpg	855.23	J/mol×K	881.91	Joback Method
cpg	868.10	J/mol×K	912.54	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=U321869&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