L-Leucine, N-methyl-N-(hexyloxycarbonyl)-, isobutyl ester

Inchi: InChI=1S/C18H35NO4/c1-7-8-9-10-11-22-18(21)19(6)16(12-14(2)3)17(20)23-13-15(4)5/h
InchiKey: UGTSMOUCBPYTKW-MRXNPFEDSA-N
Formula: C18H35NO4
SMILES: CCCCCCOC(=O)N(C)C(CC(C)C)C(=O)OCC(C)C
Mol. weight [g/mol]: 329.47

Physical Properties

Property code	Value	Unit	Source
gf	-263.70	kJ/mol	Joback Method
hf	-852.76	kJ/mol	Joback Method
hfus	40.40	kJ/mol	Joback Method
hvap	74.85	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	4.249		Crippen Method
mcvol	289.340	ml/mol	McGowan Method
pc	1246.85	kPa	Joback Method
rinpol	1979.00		NIST Webbook
rinpol	1979.00		NIST Webbook
tb	774.94	K	Joback Method
tc	958.23	K	Joback Method
tf	424.41	K	Joback Method
vc	1.091	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	893.48	J/mol×K	774.94	Joback Method
cpg	911.45	J/mol×K	805.49	Joback Method
cpg	928.40	J/mol×K	836.04	Joback Method
cpg	944.34	J/mol×K	866.58	Joback Method
cpg	959.30	J/mol×K	897.13	Joback Method
cpg	973.28	J/mol×K	927.68	Joback Method
cpg	986.32	J/mol×K	958.23	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=U392358&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