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

Inchi: InChI=1S/C17H33NO4/c1-6-8-9-10-12-22-17(20)18(5)15(13-14(3)4)16(19)21-11-7-2/h14

InchiKey: XADIKNXCJOPSPT-OAHLLOKOSA-N

Formula: C17H33NO4

SMILES: CCCCCCOC(=O)N(C)C(CC(C)C)C(=O)OCCC

Mol. weight [g/mol]: 315.45

Physical Properties

Property code	Value	Unit	Source
gf	-269.68	kJ/mol	Joback Method
hf	-826.84	kJ/mol	Joback Method
hfus	41.33	kJ/mol	Joback Method
hvap	73.02	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	4.003		Crippen Method
mcvol	275.250	ml/mol	McGowan Method
pc	1328.10	kPa	Joback Method
rinpol	1885.00		NIST Webbook
rinpol	1885.00		NIST Webbook
tb	752.50	K	Joback Method
tc	933.04	K	Joback Method
tf	428.14	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	834.02	J/mol×K	752.50	Joback Method
cpg	851.50	J/mol×K	782.59	Joback Method
cpg	868.03	J/mol×K	812.68	Joback Method
cpg	883.63	J/mol×K	842.77	Joback Method
cpg	898.30	J/mol×K	872.86	Joback Method
cpg	912.07	J/mol×K	902.95	Joback Method
cpg	924.95	J/mol×K	933.04	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=U392345&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