L-Leucine, N-allyloxycarbonyl-N-methyl-, isohexyl ester

Inchi: InChI=1S/C17H31NO4/c1-7-10-22-17(20)18(6)15(12-14(4)5)16(19)21-11-8-9-13(2)3/h7,1

InchiKey: WYBIQOWOULITPS-UHFFFAOYSA-N

Formula: C17H31NO4

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

Mol. weight [g/mol]: 313.44

Physical Properties

Property code	Value	Unit	Source
hfus	36.53	kJ/mol	Joback Method
logp	3.635		Crippen Method
mcvol	270.950	ml/mol	McGowan Method
rinpol	1868.00		NIST Webbook
rinpol	1868.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	809.00	J/mol×K	748.74	Joback Method
cpg	826.16	J/mol×K	779.36	Joback Method
cpg	842.35	J/mol×K	809.98	Joback Method
cpg	857.60	J/mol×K	840.60	Joback Method
cpg	871.93	J/mol×K	871.22	Joback Method
cpg	885.36	J/mol×K	901.84	Joback Method
cpg	897.90	J/mol×K	932.46	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U321898&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices