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

Inchi: InChI=1S/C21H33NO4/c1-16(2)10-9-13-25-20(23)19(14-17(3)4)22(5)21(24)26-15-18-11-

InchiKey: CXFHWECVKHOBHH-UHFFFAOYSA-N

Formula: C21H33NO4

SMILES: CC(C)CCCOC(=O)C(CC(C)C)N(C)C(=O)OCc1ccccc1

Mol. weight [g/mol]: 363.50

Physical Properties

Property code	Value	Unit	Source
hfus	42.21	kJ/mol	Joback Method
log10ws	-4.44		Cheméo Relay (1.0)
logp	4.649		Crippen Method
mcvol	307.850	ml/mol	McGowan Method
rinpol	2330.00		NIST Webbook
rinpol	2330.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	982.01	J/mol×K	870.26	Joback Method
cpg	998.74	J/mol×K	904.43	Joback Method
cpg	1014.19	J/mol×K	938.60	Joback Method
cpg	1028.42	J/mol×K	972.78	Joback Method
cpg	1041.45	J/mol×K	1006.95	Joback Method
cpg	1053.34	J/mol×K	1041.12	Joback Method
cpg	1064.11	J/mol×K	1075.29	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U322039&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):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices