L-leucine, n-isobutoxycarbonyl-n-methyl-, nonyl ester

Inchi: InChI=1S/C21H41NO4/c1-7-8-9-10-11-12-13-14-25-20(23)19(15-17(2)3)22(6)21(24)26-1

InchiKey: VPKCGZNXNDUMFX-UHFFFAOYSA-N

Formula: C21H41NO4

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

Mol. weight [g/mol]: 371.56

Physical Properties

Property code	Value	Unit	Source
hf	-1068.12	kJ/mol	Cheméo Relay (1.0)
hfus	48.17	kJ/mol	Joback Method
hvap	98.48	kJ/mol	Cheméo Relay (1.0)
log10ws	-5.15		Cheméo Relay (1.0)
logp	5.419		Crippen Method
mcvol	331.610	ml/mol	McGowan Method
rinpol	2245.00		NIST Webbook
tb	618.55	K	Cheméo Relay (1.0)
tf	261.04	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1075.42	J/mol×K	843.58	Joback Method
cpg	1094.38	J/mol×K	875.35	Joback Method
cpg	1112.13	J/mol×K	907.11	Joback Method
cpg	1128.71	J/mol×K	938.88	Joback Method
cpg	1144.15	J/mol×K	970.64	Joback Method
cpg	1158.47	J/mol×K	1002.41	Joback Method
cpg	1171.70	J/mol×K	1034.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321875&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point