L-Leucine, N-isobutoxycarbonyl-N-methyl-, octyl ester

Inchi: InChI=1S/C20H39NO4/c1-7-8-9-10-11-12-13-24-19(22)18(14-16(2)3)21(6)20(23)25-15-1

InchiKey: FERXWYXZZDLKNY-UHFFFAOYSA-N

Formula: C20H39NO4

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

Mol. weight [g/mol]: 357.53

Physical Properties

Property code	Value	Unit	Source
hf	-1048.11	kJ/mol	Cheméo Relay (1.0)
hfus	45.58	kJ/mol	Joback Method
hvap	94.33	kJ/mol	Cheméo Relay (1.0)
log10ws	-4.82		Cheméo Relay (1.0)
logp	5.029		Crippen Method
mcvol	317.520	ml/mol	McGowan Method
rinpol	2151.00		NIST Webbook
rinpol	2151.00		NIST Webbook
tb	611.16	K	Cheméo Relay (1.0)
tf	257.03	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1014.01	J/mol×K	820.70	Joback Method
cpg	1032.62	J/mol×K	851.94	Joback Method
cpg	1050.10	J/mol×K	883.17	Joback Method
cpg	1066.47	J/mol×K	914.41	Joback Method
cpg	1081.75	J/mol×K	945.64	Joback Method
cpg	1095.97	J/mol×K	976.88	Joback Method
cpg	1109.16	J/mol×K	1008.12	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321874&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
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