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

Inchi: InChI=1S/C18H35NO4/c1-6-8-9-10-11-12-13-23-17(20)16(14-15(3)4)19(5)18(21)22-7-2/h
InchiKey: JDWPAESHZQQJEL-UHFFFAOYSA-N
Formula: C18H35NO4
SMILES: CCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCC
Mol. weight [g/mol]: 329.48

Physical Properties

Property code	Value	Unit	Source
hf	-994.99	kJ/mol	Cheméo Relay (1.0)
hfus	43.92	kJ/mol	Joback Method
hvap	93.54	kJ/mol	Cheméo Relay (1.0)
log10ws	-4.23		Cheméo Relay (1.0)
logp	4.393		Crippen Method
mcvol	289.340	ml/mol	McGowan Method
rinpol	2034.00		NIST Webbook
tb	596.37	K	Cheméo Relay (1.0)
tf	253.23	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	892.99	J/mol×K	775.38	Joback Method
cpg	910.82	J/mol×K	805.70	Joback Method
cpg	927.65	J/mol×K	836.01	Joback Method
cpg	943.49	J/mol×K	866.33	Joback Method
cpg	958.38	J/mol×K	896.65	Joback Method
cpg	972.31	J/mol×K	926.96	Joback Method
cpg	985.32	J/mol×K	957.28	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321924&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