L-Leucine, N-methyl-N-propoxycarbonyl-, propyl ester

Inchi: InChI=1S/C14H27NO4/c1-6-8-18-13(16)12(10-11(3)4)15(5)14(17)19-9-7-2/h11-12H,6-10

InchiKey: HLLRREYNPZXPJV-UHFFFAOYSA-N

Formula: C14H27NO4

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

Mol. weight [g/mol]: 273.37

Physical Properties

Property code	Value	Unit	Source
hfus	33.56	kJ/mol	Joback Method
hvap	76.71	kJ/mol	Cheméo Relay (1.0)
logp	2.833		Crippen Method
mcvol	232.980	ml/mol	McGowan Method
pc	1657.84	kPa	Joback Method
rinpol	1645.00		NIST Webbook
rinpol	1645.00		NIST Webbook
tb	564.91	K	Cheméo Relay (1.0)
tc	721.64	K	Cheméo Relay (1.0)
tf	237.94	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	663.21	J/mol×K	683.86	Joback Method
cpg	679.58	J/mol×K	713.83	Joback Method
cpg	695.13	J/mol×K	743.81	Joback Method
cpg	709.86	J/mol×K	773.78	Joback Method
cpg	723.78	J/mol×K	803.75	Joback Method
cpg	736.90	J/mol×K	833.73	Joback Method
cpg	749.25	J/mol×K	863.70	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321853&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

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point