l-Leucine, N-allyloxycarbonyl-N-methyl-, pentyl ester

Inchi: InChI=1S/C16H29NO4/c1-6-8-9-11-20-15(18)14(12-13(3)4)17(5)16(19)21-10-7-2/h7,13-1

InchiKey: YMJQRSDWEVIPLC-UHFFFAOYSA-N

Formula: C16H29NO4

SMILES: C=CCOC(=O)N(C)C(CC(C)C)C(=O)OCCCCC

Mol. weight [g/mol]: 299.41

Physical Properties

Property code	Value	Unit	Source
gf	-190.26	kJ/mol	Joback Method
hf	-680.77	kJ/mol	Joback Method
hfus	37.46	kJ/mol	Joback Method
hvap	70.12	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	3.389		Crippen Method
mcvol	256.860	ml/mol	McGowan Method
pc	1472.49	kPa	Joback Method
rinpol	1820.00		NIST Webbook
tb	726.30	K	Joback Method
tc	907.75	K	Joback Method
tf	415.11	K	Joback Method
vc	0.967	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	751.11	J/mol×K	726.30	Joback Method
cpg	767.73	J/mol×K	756.54	Joback Method
cpg	783.46	J/mol×K	786.78	Joback Method
cpg	798.31	J/mol×K	817.02	Joback Method
cpg	812.30	J/mol×K	847.26	Joback Method
cpg	825.44	J/mol×K	877.51	Joback Method
cpg	837.76	J/mol×K	907.75	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321897&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
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
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume