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

Inchi: InChI=1S/C18H33NO4/c1-6-8-9-10-11-13-22-17(20)16(14-15(3)4)19(5)18(21)23-12-7-2/h

InchiKey: WKAIQNWAECFCCK-UHFFFAOYSA-N

Formula: C18H33NO4

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

Mol. weight [g/mol]: 327.46

Physical Properties

Property code	Value	Unit	Source
gf	-173.42	kJ/mol	Joback Method
hf	-722.05	kJ/mol	Joback Method
hfus	42.64	kJ/mol	Joback Method
hvap	74.57	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	4.169		Crippen Method
mcvol	285.040	ml/mol	McGowan Method
pc	1277.33	kPa	Joback Method
rinpol	2011.00		NIST Webbook
rinpol	2011.00		NIST Webbook
tb	772.06	K	Joback Method
tc	954.99	K	Joback Method
tf	437.65	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	866.89	J/mol×K	772.06	Joback Method
cpg	884.20	J/mol×K	802.55	Joback Method
cpg	900.54	J/mol×K	833.04	Joback Method
cpg	915.92	J/mol×K	863.52	Joback Method
cpg	930.36	J/mol×K	894.01	Joback Method
cpg	943.89	J/mol×K	924.50	Joback Method
cpg	956.52	J/mol×K	954.99	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321900&Units=SI

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