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

Inchi: InChI=1S/C14H25NO4/c1-6-8-18-13(16)12(10-11(3)4)15(5)14(17)19-9-7-2/h7,11-12H,2,
InchiKey: LIFVPMZSQXEDOD-UHFFFAOYSA-N
Formula: C14H25NO4
SMILES: C=CCOC(=O)N(C)C(CC(C)C)C(=O)OCCC
Mol. weight [g/mol]: 271.35

Physical Properties

Property code	Value	Unit	Source
gf	-207.10	kJ/mol	Joback Method
hf	-639.49	kJ/mol	Joback Method
hfus	32.28	kJ/mol	Joback Method
hvap	65.67	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	2.609		Crippen Method
mcvol	228.680	ml/mol	McGowan Method
pc	1716.03	kPa	Joback Method
rinpol	1645.00		NIST Webbook
rinpol	1645.00		NIST Webbook
tb	680.54	K	Joback Method
tc	862.63	K	Joback Method
tf	392.57	K	Joback Method
vc	0.855	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	639.61	J/mol×K	680.54	Joback Method
cpg	655.47	J/mol×K	710.89	Joback Method
cpg	670.50	J/mol×K	741.24	Joback Method
cpg	684.73	J/mol×K	771.58	Joback Method
cpg	698.16	J/mol×K	801.93	Joback Method
cpg	710.80	J/mol×K	832.28	Joback Method
cpg	722.68	J/mol×K	862.63	Joback Method

Sources

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=U321896&Units=SI
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
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