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

Inchi: InChI=1S/C14H23NO4/c1-6-8-18-13(16)12(10-11(3)4)15(5)14(17)19-9-7-2/h6-7,11-12H,

InchiKey: NTZQHYDFDGPPRC-UHFFFAOYSA-N

Formula: C14H23NO4

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

Mol. weight [g/mol]: 269.34

Physical Properties

Property code	Value	Unit	Source
gf	-119.26	kJ/mol	Joback Method
hf	-514.06	kJ/mol	Joback Method
hfus	31.00	kJ/mol	Joback Method
hvap	65.00	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	2.385		Crippen Method
mcvol	224.380	ml/mol	McGowan Method
pc	1777.34	kPa	Joback Method
rinpol	1628.00		NIST Webbook
rinpol	1628.00		NIST Webbook
tb	677.22	K	Joback Method
tc	861.71	K	Joback Method
tf	390.81	K	Joback Method
vc	0.836	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	616.18	J/mol×K	677.22	Joback Method
cpg	631.51	J/mol×K	707.97	Joback Method
cpg	646.02	J/mol×K	738.72	Joback Method
cpg	659.73	J/mol×K	769.47	Joback Method
cpg	672.66	J/mol×K	800.21	Joback Method
cpg	684.82	J/mol×K	830.96	Joback Method
cpg	696.22	J/mol×K	861.71	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=U321908&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