L-Leucine, N-methyl-N-(2-(benzyloxy)ethoxycarbonyl)-, undecyl ester

Inchi: InChI=1S/C28H47NO5/c1-5-6-7-8-9-10-11-12-16-19-33-27(30)26(22-24(2)3)29(4)28(31)
InchiKey: PIGDPYGLMCUXAH-AREMUKBSSA-N
Formula: C28H47NO5
SMILES: CCCCCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCCOCc1ccccc1
Mol. weight [g/mol]: 477.68

Physical Properties

Property code	Value	Unit	Source
gf	-169.65	kJ/mol	Joback Method
hf	-949.57	kJ/mol	Joback Method
hfus	65.05	kJ/mol	Joback Method
hvap	102.19	kJ/mol	Joback Method
log10ws	-7.37		Crippen Method
logp	6.760		Crippen Method
mcvol	412.350	ml/mol	McGowan Method
pc	822.90	kPa	Joback Method
rinpol	3105.00		NIST Webbook
rinpol	3105.00		NIST Webbook
tb	1053.28	K	Joback Method
tc	1297.27	K	Joback Method
tf	600.76	K	Joback Method
vc	1.567	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1443.86	J/mol×K	1053.28	Joback Method
cpg	1461.14	J/mol×K	1093.95	Joback Method
cpg	1476.38	J/mol×K	1134.61	Joback Method
cpg	1489.65	J/mol×K	1175.28	Joback Method
cpg	1501.04	J/mol×K	1215.94	Joback Method
cpg	1510.63	J/mol×K	1256.61	Joback Method
cpg	1518.50	J/mol×K	1297.27	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=U392371&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