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

Inchi: InChI=1S/C29H49NO5/c1-5-6-7-8-9-10-11-12-13-17-20-34-28(31)27(23-25(2)3)30(4)29(3
InchiKey: LPWSGAITAZLTGG-HHHXNRCGSA-N
Formula: C29H49NO5
SMILES: CCCCCCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCCOCc1ccccc1
Mol. weight [g/mol]: 491.70

Physical Properties

Property code	Value	Unit	Source
gf	-161.23	kJ/mol	Joback Method
hf	-970.21	kJ/mol	Joback Method
hfus	67.64	kJ/mol	Joback Method
hvap	104.41	kJ/mol	Joback Method
log10ws	-7.79		Crippen Method
logp	7.150		Crippen Method
mcvol	426.440	ml/mol	McGowan Method
pc	779.38	kPa	Joback Method
rinpol	3206.00		NIST Webbook
rinpol	3206.00		NIST Webbook
tb	1076.16	K	Joback Method
tc	1330.37	K	Joback Method
tf	612.03	K	Joback Method
vc	1.623	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1507.00	J/mol×K	1076.16	Joback Method
cpg	1524.54	J/mol×K	1118.53	Joback Method
cpg	1539.86	J/mol×K	1160.90	Joback Method
cpg	1553.06	J/mol×K	1203.26	Joback Method
cpg	1564.23	J/mol×K	1245.63	Joback Method
cpg	1573.48	J/mol×K	1288.00	Joback Method
cpg	1580.91	J/mol×K	1330.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392372&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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