l-Leucine, N-benzyloxycarbonyl-N-methyl-, dodecyl ester

Inchi: InChI=1S/C27H45NO4/c1-5-6-7-8-9-10-11-12-13-17-20-31-26(29)25(21-23(2)3)28(4)27(
InchiKey: MKOLRNGGSWISLE-UHFFFAOYSA-N
Formula: C27H45NO4
SMILES: CCCCCCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCc1ccccc1
Mol. weight [g/mol]: 447.65

Physical Properties

Property code	Value	Unit	Source
gf	-73.07	kJ/mol	Joback Method
hf	-796.71	kJ/mol	Joback Method
hfus	61.28	kJ/mol	Joback Method
hvap	97.55	kJ/mol	Joback Method
log10ws	-7.87		Crippen Method
logp	7.134		Crippen Method
mcvol	392.390	ml/mol	McGowan Method
pc	878.96	kPa	Joback Method
rinpol	3062.00		NIST Webbook
tb	1007.98	K	Joback Method
tc	1235.82	K	Joback Method
tf	567.26	K	Joback Method
vc	1.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1351.89	J/mol×K	1007.98	Joback Method
cpg	1369.84	J/mol×K	1045.95	Joback Method
cpg	1386.15	J/mol×K	1083.93	Joback Method
cpg	1400.90	J/mol×K	1121.90	Joback Method
cpg	1414.17	J/mol×K	1159.87	Joback Method
cpg	1426.04	J/mol×K	1197.85	Joback Method
cpg	1436.59	J/mol×K	1235.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U322043&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

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