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

Inchi: InChI=1S/C27H45NO5/c1-5-6-7-8-9-10-11-15-18-32-26(29)25(21-23(2)3)28(4)27(30)33-
InchiKey: MEHHRXQBYNFBNU-RUZDIDTESA-N
Formula: C27H45NO5
SMILES: CCCCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCCOCc1ccccc1
Mol. weight [g/mol]: 463.65

Physical Properties

Property code	Value	Unit	Source
gf	-178.07	kJ/mol	Joback Method
hf	-928.93	kJ/mol	Joback Method
hfus	62.46	kJ/mol	Joback Method
hvap	99.96	kJ/mol	Joback Method
log10ws	-6.95		Crippen Method
logp	6.370		Crippen Method
mcvol	398.260	ml/mol	McGowan Method
pc	870.16	kPa	Joback Method
rinpol	3005.00		NIST Webbook
rinpol	3005.00		NIST Webbook
tb	1030.40	K	Joback Method
tc	1265.53	K	Joback Method
tf	589.49	K	Joback Method
vc	1.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1380.97	J/mol×K	1030.40	Joback Method
cpg	1398.02	J/mol×K	1069.59	Joback Method
cpg	1413.17	J/mol×K	1108.78	Joback Method
cpg	1426.49	J/mol×K	1147.96	Joback Method
cpg	1438.06	J/mol×K	1187.15	Joback Method
cpg	1447.93	J/mol×K	1226.34	Joback Method
cpg	1456.19	J/mol×K	1265.53	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=U392370&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