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

Inchi: InChI=1S/C25H41NO5/c1-5-6-7-8-9-13-16-30-24(27)23(19-21(2)3)26(4)25(28)31-18-17-2
InchiKey: XDAAPJLMJDIPTG-HSZRJFAPSA-N
Formula: C25H41NO5
SMILES: CCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCCOCc1ccccc1
Mol. weight [g/mol]: 435.60

Physical Properties

Property code	Value	Unit	Source
gf	-194.91	kJ/mol	Joback Method
hf	-887.65	kJ/mol	Joback Method
hfus	57.28	kJ/mol	Joback Method
hvap	95.51	kJ/mol	Joback Method
log10ws	-6.12		Crippen Method
logp	5.590		Crippen Method
mcvol	370.080	ml/mol	McGowan Method
pc	977.78	kPa	Joback Method
rinpol	2809.00		NIST Webbook
rinpol	2809.00		NIST Webbook
tb	984.64	K	Joback Method
tc	1205.73	K	Joback Method
tf	566.95	K	Joback Method
vc	1.399	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1256.08	J/mol×K	984.64	Joback Method
cpg	1272.72	J/mol×K	1021.49	Joback Method
cpg	1287.71	J/mol×K	1058.34	Joback Method
cpg	1301.09	J/mol×K	1095.19	Joback Method
cpg	1312.92	J/mol×K	1132.04	Joback Method
cpg	1323.25	J/mol×K	1168.88	Joback Method
cpg	1332.13	J/mol×K	1205.73	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=U392368&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