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

Inchi: InChI=1S/C26H35NO6/c1-21(2)18-24(25(28)32-16-14-30-19-22-10-6-4-7-11-22)27(3)26(
InchiKey: HAOSXWJKNOWILL-XMMPIXPASA-N
Formula: C26H35NO6
SMILES: CC(C)CC(C(=O)OCCOCc1ccccc1)N(C)C(=O)OCCOCc1ccccc1
Mol. weight [g/mol]: 457.56

Physical Properties

Property code	Value	Unit	Source
gf	-179.08	kJ/mol	Joback Method
hf	-803.98	kJ/mol	Joback Method
hfus	55.10	kJ/mol	Joback Method
hvap	102.42	kJ/mol	Joback Method
log10ws	-5.22		Crippen Method
logp	4.446		Crippen Method
mcvol	366.280	ml/mol	McGowan Method
pc	1126.08	kPa	Joback Method
rinpol	3162.00		NIST Webbook
rinpol	3162.00		NIST Webbook
tb	1056.62	K	Joback Method
tc	1293.63	K	Joback Method
tf	626.87	K	Joback Method
vc	1.365	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1235.77	J/mol×K	1056.62	Joback Method
cpg	1248.05	J/mol×K	1096.12	Joback Method
cpg	1258.44	J/mol×K	1135.62	Joback Method
cpg	1267.01	J/mol×K	1175.12	Joback Method
cpg	1273.81	J/mol×K	1214.63	Joback Method
cpg	1278.88	J/mol×K	1254.13	Joback Method
cpg	1282.30	J/mol×K	1293.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392373&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