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

Inchi: InChI=1S/C26H43NO5/c1-5-6-7-8-9-10-14-17-31-25(28)24(20-22(2)3)27(4)26(29)32-19-
InchiKey: GGDNSOVBEHVBJT-XMMPIXPASA-N
Formula: C26H43NO5
SMILES: CCCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCCOCc1ccccc1
Mol. weight [g/mol]: 449.62

Physical Properties

Property code	Value	Unit	Source
gf	-186.49	kJ/mol	Joback Method
hf	-908.29	kJ/mol	Joback Method
hfus	59.87	kJ/mol	Joback Method
hvap	97.73	kJ/mol	Joback Method
log10ws	-6.53		Crippen Method
logp	5.980		Crippen Method
mcvol	384.170	ml/mol	McGowan Method
pc	921.62	kPa	Joback Method
rinpol	2904.00		NIST Webbook
rinpol	2904.00		NIST Webbook
tb	1007.52	K	Joback Method
tc	1235.05	K	Joback Method
tf	578.22	K	Joback Method
vc	1.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1318.36	J/mol×K	1007.52	Joback Method
cpg	1335.19	J/mol×K	1045.44	Joback Method
cpg	1350.26	J/mol×K	1083.36	Joback Method
cpg	1363.62	J/mol×K	1121.28	Joback Method
cpg	1375.33	J/mol×K	1159.20	Joback Method
cpg	1385.45	J/mol×K	1197.12	Joback Method
cpg	1394.05	J/mol×K	1235.05	Joback Method

Sources

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=U392369&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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