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

Inchi: InChI=1S/C24H39NO4/c1-5-6-7-8-9-10-14-17-28-23(26)22(18-20(2)3)25(4)24(27)29-19-
InchiKey: CYLPPLIOBHQTOQ-UHFFFAOYSA-N
Formula: C24H39NO4
SMILES: CCCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCc1ccccc1
Mol. weight [g/mol]: 405.57

Physical Properties

Property code	Value	Unit	Source
gf	-98.33	kJ/mol	Joback Method
hf	-734.79	kJ/mol	Joback Method
hfus	53.51	kJ/mol	Joback Method
hvap	90.87	kJ/mol	Joback Method
log10ws	-6.61		Crippen Method
logp	5.963		Crippen Method
mcvol	350.120	ml/mol	McGowan Method
pc	1050.73	kPa	Joback Method
rinpol	2673.00		NIST Webbook
tb	939.34	K	Joback Method
tc	1150.73	K	Joback Method
tf	533.45	K	Joback Method
vc	1.325	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1164.45	J/mol×K	939.34	Joback Method
cpg	1181.61	J/mol×K	974.57	Joback Method
cpg	1197.38	J/mol×K	1009.80	Joback Method
cpg	1211.81	J/mol×K	1045.03	Joback Method
cpg	1224.95	J/mol×K	1080.27	Joback Method
cpg	1236.85	J/mol×K	1115.50	Joback Method
cpg	1247.58	J/mol×K	1150.73	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=U322041&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

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