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

Inchi: InChI=1S/C20H31NO4/c1-5-6-10-13-24-19(22)18(14-16(2)3)21(4)20(23)25-15-17-11-8-7

InchiKey: CCVPWMKBKLCZHY-UHFFFAOYSA-N

Formula: C20H31NO4

SMILES: CCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCc1ccccc1

Mol. weight [g/mol]: 349.46

Physical Properties

Property code	Value	Unit	Source
gf	-132.01	kJ/mol	Joback Method
hf	-652.23	kJ/mol	Joback Method
hfus	43.15	kJ/mol	Joback Method
hvap	81.97	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.403		Crippen Method
mcvol	293.760	ml/mol	McGowan Method
pc	1370.73	kPa	Joback Method
rinpol	2295.00		NIST Webbook
rinpol	2295.00		NIST Webbook
tb	847.82	K	Joback Method
tc	1050.34	K	Joback Method
tf	488.37	K	Joback Method
vc	1.101	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	921.80	J/mol×K	847.82	Joback Method
cpg	938.27	J/mol×K	881.57	Joback Method
cpg	953.54	J/mol×K	915.33	Joback Method
cpg	967.63	J/mol×K	949.08	Joback Method
cpg	980.60	J/mol×K	982.84	Joback Method
cpg	992.47	J/mol×K	1016.59	Joback Method
cpg	1003.28	J/mol×K	1050.34	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=U322038&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