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

Inchi: InChI=1S/C18H27NO4/c1-5-11-22-17(20)16(12-14(2)3)19(4)18(21)23-13-15-9-7-6-8-10-

InchiKey: CJXDJBLTLCKPTQ-UHFFFAOYSA-N

Formula: C18H27NO4

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

Mol. weight [g/mol]: 321.41

Physical Properties

Property code	Value	Unit	Source
gf	-148.85	kJ/mol	Joback Method
hf	-610.95	kJ/mol	Joback Method
hfus	37.97	kJ/mol	Joback Method
hvap	77.52	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	3.623		Crippen Method
mcvol	265.580	ml/mol	McGowan Method
pc	1588.54	kPa	Joback Method
rinpol	2118.00		NIST Webbook
rinpol	2118.00		NIST Webbook
tb	802.06	K	Joback Method
tc	1004.66	K	Joback Method
tf	465.83	K	Joback Method
vc	0.990	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	804.62	J/mol×K	802.06	Joback Method
cpg	820.78	J/mol×K	835.83	Joback Method
cpg	835.79	J/mol×K	869.59	Joback Method
cpg	849.68	J/mol×K	903.36	Joback Method
cpg	862.50	J/mol×K	937.13	Joback Method
cpg	874.26	J/mol×K	970.90	Joback Method
cpg	885.01	J/mol×K	1004.66	Joback Method

Sources

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=U322035&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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