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

Inchi: InChI=1S/C21H33NO4/c1-5-6-7-11-14-25-20(23)19(15-17(2)3)22(4)21(24)26-16-18-12-9

InchiKey: DIWVROZPZOBSPP-UHFFFAOYSA-N

Formula: C21H33NO4

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

Mol. weight [g/mol]: 363.49

Physical Properties

Property code	Value	Unit	Source
gf	-123.59	kJ/mol	Joback Method
hf	-672.87	kJ/mol	Joback Method
hfus	45.74	kJ/mol	Joback Method
hvap	84.19	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.793		Crippen Method
mcvol	307.850	ml/mol	McGowan Method
pc	1278.25	kPa	Joback Method
rinpol	2388.00		NIST Webbook
rinpol	2388.00		NIST Webbook
tb	870.70	K	Joback Method
tc	1074.23	K	Joback Method
tf	499.64	K	Joback Method
vc	1.157	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	981.52	J/mol×K	870.70	Joback Method
cpg	998.14	J/mol×K	904.62	Joback Method
cpg	1013.53	J/mol×K	938.54	Joback Method
cpg	1027.70	J/mol×K	972.47	Joback Method
cpg	1040.72	J/mol×K	1006.39	Joback Method
cpg	1052.62	J/mol×K	1040.31	Joback Method
cpg	1063.43	J/mol×K	1074.23	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=U322040&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