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

Inchi: InChI=1S/C17H25NO4/c1-5-21-16(19)15(11-13(2)3)18(4)17(20)22-12-14-9-7-6-8-10-14/l

InchiKey: RDLCNYDMNHUZEM-UHFFFAOYSA-N

Formula: C17H25NO4

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

Mol. weight [g/mol]: 307.38

Physical Properties

Property code	Value	Unit	Source
gf	-157.27	kJ/mol	Joback Method
hf	-590.31	kJ/mol	Joback Method
hfus	35.38	kJ/mol	Joback Method
hvap	75.29	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.233		Crippen Method
mcvol	251.490	ml/mol	McGowan Method
pc	1717.45	kPa	Joback Method
rinpol	2042.00		NIST Webbook
rinpol	2042.00		NIST Webbook
tb	779.18	K	Joback Method
tc	982.77	K	Joback Method
tf	454.56	K	Joback Method
vc	0.933	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	747.29	J/mol×K	779.18	Joback Method
cpg	763.27	J/mol×K	813.11	Joback Method
cpg	778.12	J/mol×K	847.04	Joback Method
cpg	791.89	J/mol×K	880.97	Joback Method
cpg	804.60	J/mol×K	914.90	Joback Method
cpg	816.27	J/mol×K	948.84	Joback Method
cpg	826.95	J/mol×K	982.77	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=U322034&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