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

Inchi: InChI=1S/C17H33NO4/c1-7-8-9-10-21-16(19)15(11-13(2)3)18(6)17(20)22-12-14(4)5/h13

InchiKey: OZJQDLALJWAQKT-UHFFFAOYSA-N

Formula: C17H33NO4

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

Mol. weight [g/mol]: 315.45

Physical Properties

Property code	Value	Unit	Source
gf	-272.12	kJ/mol	Joback Method
hf	-832.12	kJ/mol	Joback Method
hfus	37.81	kJ/mol	Joback Method
hvap	72.63	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.859		Crippen Method
mcvol	275.250	ml/mol	McGowan Method
pc	1335.88	kPa	Joback Method
rinpol	1873.00		NIST Webbook
rinpol	1873.00		NIST Webbook
tb	752.06	K	Joback Method
tc	934.27	K	Joback Method
tf	413.14	K	Joback Method
vc	1.036	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	834.50	J/mol×K	752.06	Joback Method
cpg	852.16	J/mol×K	782.43	Joback Method
cpg	868.84	J/mol×K	812.80	Joback Method
cpg	884.56	J/mol×K	843.17	Joback Method
cpg	899.33	J/mol×K	873.53	Joback Method
cpg	913.18	J/mol×K	903.90	Joback Method
cpg	926.11	J/mol×K	934.27	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=U321870&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