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

Inchi: InChI=1S/C18H35NO4/c1-13(2)9-8-10-22-17(20)16(11-14(3)4)19(7)18(21)23-12-15(5)6/h

InchiKey: VZOJBEAVPYCAGU-UHFFFAOYSA-N

Formula: C18H35NO4

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

Mol. weight [g/mol]: 329.47

Physical Properties

Property code	Value	Unit	Source
gf	-266.14	kJ/mol	Joback Method
hf	-858.04	kJ/mol	Joback Method
hfus	36.88	kJ/mol	Joback Method
hvap	74.46	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	4.105		Crippen Method
mcvol	289.340	ml/mol	McGowan Method
pc	1253.92	kPa	Joback Method
rinpol	1926.00		NIST Webbook
rinpol	1926.00		NIST Webbook
tb	774.50	K	Joback Method
tc	959.30	K	Joback Method
tf	409.41	K	Joback Method
vc	1.085	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	893.96	J/mol×K	774.50	Joback Method
cpg	912.09	J/mol×K	805.30	Joback Method
cpg	929.17	J/mol×K	836.10	Joback Method
cpg	945.22	J/mol×K	866.90	Joback Method
cpg	960.26	J/mol×K	897.70	Joback Method
cpg	974.30	J/mol×K	928.50	Joback Method
cpg	987.37	J/mol×K	959.30	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=U321871&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

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