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

Inchi: InChI=1S/C19H37NO4/c1-14(2)10-9-11-23-17(21)16(12-15(3)4)20(8)18(22)24-13-19(5,6

InchiKey: FVMCSSMKMYAECS-UHFFFAOYSA-N

Formula: C19H37NO4

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

Mol. weight [g/mol]: 343.50

Physical Properties

Property code	Value	Unit	Source
gf	-252.44	kJ/mol	Joback Method
hf	-882.15	kJ/mol	Joback Method
hfus	35.58	kJ/mol	Joback Method
hvap	75.78	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	4.495		Crippen Method
mcvol	303.430	ml/mol	McGowan Method
pc	1181.71	kPa	Joback Method
rinpol	1960.00		NIST Webbook
rinpol	1960.00		NIST Webbook
tb	794.59	K	Joback Method
tc	983.17	K	Joback Method
tf	438.10	K	Joback Method
vc	1.137	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	954.48	J/mol×K	794.59	Joback Method
cpg	972.88	J/mol×K	826.02	Joback Method
cpg	990.18	J/mol×K	857.45	Joback Method
cpg	1006.40	J/mol×K	888.88	Joback Method
cpg	1021.59	J/mol×K	920.31	Joback Method
cpg	1035.78	J/mol×K	951.74	Joback Method
cpg	1049.01	J/mol×K	983.17	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=U321909&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