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

Inchi: InChI=1S/C31H61NO4/c1-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-35-29(33

InchiKey: FVRVHXRXWMENTN-UHFFFAOYSA-N

Formula: C31H61NO4

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

Mol. weight [g/mol]: 511.82

Physical Properties

Property code	Value	Unit	Source
gf	-148.96	kJ/mol	Joback Method
hf	-1124.55	kJ/mol	Joback Method
hfus	70.18	kJ/mol	Joback Method
hvap	102.88	kJ/mol	Joback Method
log10ws	-9.70		Crippen Method
logp	9.320		Crippen Method
mcvol	472.510	ml/mol	McGowan Method
pc	603.98	kPa	Joback Method
tb	1069.59	K	Joback Method
tc	1342.29	K	Joback Method
tf	588.34	K	Joback Method
vc	1.815	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1716.67	J/mol×K	1069.59	Joback Method
cpg	1741.14	J/mol×K	1115.04	Joback Method
cpg	1763.29	J/mol×K	1160.49	Joback Method
cpg	1783.31	J/mol×K	1205.94	Joback Method
cpg	1801.38	J/mol×K	1251.39	Joback Method
cpg	1817.70	J/mol×K	1296.84	Joback Method
cpg	1832.47	J/mol×K	1342.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321919&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume