l-Leucine, N-methyl-n-propoxycarbonyl-, octyl ester

Inchi: InChI=1S/C19H37NO4/c1-6-8-9-10-11-12-14-23-18(21)17(15-16(3)4)20(5)19(22)24-13-7

InchiKey: NGMJMPMGQHOYPX-UHFFFAOYSA-N

Formula: C19H37NO4

SMILES: CCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCCC

Mol. weight [g/mol]: 343.50

Physical Properties

Property code	Value	Unit	Source
gf	-252.84	kJ/mol	Joback Method
hf	-868.12	kJ/mol	Joback Method
hfus	46.52	kJ/mol	Joback Method
hvap	77.47	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.783		Crippen Method
mcvol	303.430	ml/mol	McGowan Method
pc	1160.08	kPa	Joback Method
rinpol	2107.00		NIST Webbook
tb	798.26	K	Joback Method
tc	982.17	K	Joback Method
tf	450.68	K	Joback Method
vc	1.153	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	952.86	J/mol×K	798.26	Joback Method
cpg	971.04	J/mol×K	828.91	Joback Method
cpg	988.16	J/mol×K	859.56	Joback Method
cpg	1004.24	J/mol×K	890.22	Joback Method
cpg	1019.32	J/mol×K	920.87	Joback Method
cpg	1033.40	J/mol×K	951.52	Joback Method
cpg	1046.51	J/mol×K	982.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321858&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume