L-Leucine, N-methyl-N-(hexyloxycarbonyl)-, tridecyl ester

Inchi: InChI=1S/C27H53NO4/c1-6-8-10-12-13-14-15-16-17-18-20-21-31-26(29)25(23-24(3)4)28

InchiKey: HOQXVGGQXCGNIK-RUZDIDTESA-N

Formula: C27H53NO4

SMILES: CCCCCCCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCCCCCC

Mol. weight [g/mol]: 455.71

Physical Properties

Property code	Value	Unit	Source
gf	-185.48	kJ/mol	Joback Method
hf	-1033.24	kJ/mol	Joback Method
hfus	67.24	kJ/mol	Joback Method
hvap	95.28	kJ/mol	Joback Method
log10ws	-8.27		Crippen Method
logp	7.904		Crippen Method
mcvol	416.150	ml/mol	McGowan Method
pc	728.88	kPa	Joback Method
rinpol	2801.00		NIST Webbook
rinpol	2801.00		NIST Webbook
tb	981.30	K	Joback Method
tc	1212.75	K	Joback Method
tf	540.84	K	Joback Method
vc	1.601	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1455.55	J/mol×K	981.30	Joback Method
cpg	1477.49	J/mol×K	1019.88	Joback Method
cpg	1497.54	J/mol×K	1058.45	Joback Method
cpg	1515.78	J/mol×K	1097.03	Joback Method
cpg	1532.28	J/mol×K	1135.60	Joback Method
cpg	1547.11	J/mol×K	1174.18	Joback Method
cpg	1560.35	J/mol×K	1212.75	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=U392351&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