L-Leucine, N-methyl-N-(octyloxycarbonyl)-, isohexyl ester

Inchi: InChI=1S/C22H43NO4/c1-7-8-9-10-11-12-15-27-22(25)23(6)20(17-19(4)5)21(24)26-16-1

InchiKey: QWQUUFWQSSPWMQ-HXUWFJFHSA-N

Formula: C22H43NO4

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

Mol. weight [g/mol]: 385.58

Physical Properties

Property code	Value	Unit	Source
gf	-230.02	kJ/mol	Joback Method
hf	-935.32	kJ/mol	Joback Method
hfus	50.76	kJ/mol	Joback Method
hvap	83.76	kJ/mol	Joback Method
log10ws	-5.93		Crippen Method
logp	5.809		Crippen Method
mcvol	345.700	ml/mol	McGowan Method
pc	966.87	kPa	Joback Method
rinpol	3085.00		NIST Webbook
rinpol	3085.00		NIST Webbook
tb	866.46	K	Joback Method
tc	1061.06	K	Joback Method
tf	469.49	K	Joback Method
vc	1.315	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1137.50	J/mol×K	866.46	Joback Method
cpg	1156.82	J/mol×K	898.89	Joback Method
cpg	1174.87	J/mol×K	931.33	Joback Method
cpg	1191.67	J/mol×K	963.76	Joback Method
cpg	1207.26	J/mol×K	996.19	Joback Method
cpg	1221.67	J/mol×K	1028.62	Joback Method
cpg	1234.92	J/mol×K	1061.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392367&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