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

Inchi: InChI=1S/C21H41NO4/c1-6-8-10-11-12-14-16-26-21(24)22(5)19(17-18(3)4)20(23)25-15-

InchiKey: FFMMCHGUTRXQBP-LJQANCHMSA-N

Formula: C21H41NO4

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

Mol. weight [g/mol]: 371.55

Physical Properties

Property code	Value	Unit	Source
gf	-236.00	kJ/mol	Joback Method
hf	-909.40	kJ/mol	Joback Method
hfus	51.69	kJ/mol	Joback Method
hvap	81.92	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	5.563		Crippen Method
mcvol	331.610	ml/mol	McGowan Method
pc	1022.04	kPa	Joback Method
rinpol	3009.00		NIST Webbook
rinpol	3009.00		NIST Webbook
tb	844.02	K	Joback Method
tc	1034.17	K	Joback Method
tf	473.22	K	Joback Method
vc	1.266	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1074.95	J/mol×K	844.02	Joback Method
cpg	1093.87	J/mol×K	875.71	Joback Method
cpg	1111.61	J/mol×K	907.40	Joback Method
cpg	1128.18	J/mol×K	939.09	Joback Method
cpg	1143.62	J/mol×K	970.78	Joback Method
cpg	1157.96	J/mol×K	1002.48	Joback Method
cpg	1171.23	J/mol×K	1034.17	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392360&Units=SI

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