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

Inchi: InChI=1S/C22H43NO4/c1-8-9-10-11-12-13-14-15-26-20(24)19(16-18(2)3)23(7)21(25)27-

InchiKey: IPVIRECPSRVDAJ-UHFFFAOYSA-N

Formula: C22H43NO4

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

Mol. weight [g/mol]: 385.58

Physical Properties

Property code	Value	Unit	Source
gf	-224.74	kJ/mol	Joback Method
hf	-938.79	kJ/mol	Joback Method
hfus	46.87	kJ/mol	Joback Method
hvap	82.85	kJ/mol	Joback Method
log10ws	-5.93		Crippen Method
logp	5.809		Crippen Method
mcvol	345.700	ml/mol	McGowan Method
pc	973.52	kPa	Joback Method
rinpol	2286.00		NIST Webbook
tb	863.67	K	Joback Method
tc	1058.45	K	Joback Method
tf	486.91	K	Joback Method
vc	1.310	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1137.44	J/mol×K	863.67	Joback Method
cpg	1156.61	J/mol×K	896.13	Joback Method
cpg	1174.56	J/mol×K	928.60	Joback Method
cpg	1191.32	J/mol×K	961.06	Joback Method
cpg	1206.95	J/mol×K	993.52	Joback Method
cpg	1221.50	J/mol×K	1025.99	Joback Method
cpg	1235.01	J/mol×K	1058.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321913&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