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

Inchi: InChI=1S/C20H39NO4/c1-8-9-10-11-12-13-24-18(22)17(14-16(2)3)21(7)19(23)25-15-20(

InchiKey: MHFYZIPNTHADMH-UHFFFAOYSA-N

Formula: C20H39NO4

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

Mol. weight [g/mol]: 357.53

Physical Properties

Property code	Value	Unit	Source
gf	-241.58	kJ/mol	Joback Method
hf	-897.51	kJ/mol	Joback Method
hfus	41.69	kJ/mol	Joback Method
hvap	78.40	kJ/mol	Joback Method
log10ws	-5.10		Crippen Method
logp	5.029		Crippen Method
mcvol	317.520	ml/mol	McGowan Method
pc	1101.54	kPa	Joback Method
rinpol	2097.00		NIST Webbook
rinpol	2097.00		NIST Webbook
tb	817.91	K	Joback Method
tc	1006.82	K	Joback Method
tf	464.37	K	Joback Method
vc	1.198	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1014.41	J/mol×K	817.91	Joback Method
cpg	1032.95	J/mol×K	849.39	Joback Method
cpg	1050.36	J/mol×K	880.88	Joback Method
cpg	1066.69	J/mol×K	912.36	Joback Method
cpg	1081.98	J/mol×K	943.85	Joback Method
cpg	1096.25	J/mol×K	975.33	Joback Method
cpg	1109.56	J/mol×K	1006.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321911&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