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

Inchi: InChI=1S/C21H41NO4/c1-8-9-10-11-12-13-14-25-19(23)18(15-17(2)3)22(7)20(24)26-16-

InchiKey: XSZOBVQLLWXEKA-UHFFFAOYSA-N

Formula: C21H41NO4

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

Mol. weight [g/mol]: 371.55

Physical Properties

Property code	Value	Unit	Source
gf	-233.16	kJ/mol	Joback Method
hf	-918.15	kJ/mol	Joback Method
hfus	44.28	kJ/mol	Joback Method
hvap	80.62	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	5.419		Crippen Method
mcvol	331.610	ml/mol	McGowan Method
pc	1034.57	kPa	Joback Method
rinpol	2186.00		NIST Webbook
tb	840.79	K	Joback Method
tc	1032.24	K	Joback Method
tf	475.64	K	Joback Method
vc	1.254	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1075.58	J/mol×K	840.79	Joback Method
cpg	1094.42	J/mol×K	872.70	Joback Method
cpg	1112.09	J/mol×K	904.61	Joback Method
cpg	1128.63	J/mol×K	936.51	Joback Method
cpg	1144.08	J/mol×K	968.42	Joback Method
cpg	1158.49	J/mol×K	1000.33	Joback Method
cpg	1171.90	J/mol×K	1032.24	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=U321912&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