l-Leucine, N-isobutoxycarbonyl-N-methyl-, hexadecyl ester

Inchi: InChI=1S/C28H55NO4/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-32-27(30)26(22-2

InchiKey: WTDAKLUVIOBYBF-UHFFFAOYSA-N

Formula: C28H55NO4

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

Mol. weight [g/mol]: 469.74

Physical Properties

Property code	Value	Unit	Source
gf	-179.50	kJ/mol	Joback Method
hf	-1059.16	kJ/mol	Joback Method
hfus	66.30	kJ/mol	Joback Method
hvap	97.11	kJ/mol	Joback Method
log10ws	-8.44		Crippen Method
logp	8.150		Crippen Method
mcvol	430.240	ml/mol	McGowan Method
pc	695.45	kPa	Joback Method
rinpol	3014.00		NIST Webbook
tb	1003.74	K	Joback Method
tc	1243.81	K	Joback Method
tf	537.11	K	Joback Method
vc	1.651	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1520.75	J/mol×K	1003.74	Joback Method
cpg	1543.08	J/mol×K	1043.75	Joback Method
cpg	1563.35	J/mol×K	1083.76	Joback Method
cpg	1581.66	J/mol×K	1123.78	Joback Method
cpg	1598.09	J/mol×K	1163.79	Joback Method
cpg	1612.73	J/mol×K	1203.80	Joback Method
cpg	1625.67	J/mol×K	1243.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321879&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

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