L-Leucine, N-isobutoxycarbonyl-N-methyl-, octadecyl ester

Inchi: InChI=1S/C30H59NO4/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-34-29(32)2

InchiKey: AYKJWKHVOIPLMQ-UHFFFAOYSA-N

Formula: C30H59NO4

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

Mol. weight [g/mol]: 497.80

Physical Properties

Property code	Value	Unit	Source
hf	-1246.22	kJ/mol	Cheméo Relay (1.0)
hfus	71.48	kJ/mol	Joback Method
hvap	134.49	kJ/mol	Cheméo Relay (1.0)
log10ws	-7.97		Cheméo Relay (1.0)
logp	8.930		Crippen Method
mcvol	458.420	ml/mol	McGowan Method
rinpol	3418.00		NIST Webbook
rinpol	3418.00		NIST Webbook
tb	680.52	K	Cheméo Relay (1.0)
tf	294.51	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1651.38	J/mol×K	1049.50	Joback Method
cpg	1675.08	J/mol×K	1093.76	Joback Method
cpg	1696.29	J/mol×K	1138.02	Joback Method
cpg	1715.14	J/mol×K	1182.28	Joback Method
cpg	1731.75	J/mol×K	1226.54	Joback Method
cpg	1746.26	J/mol×K	1270.80	Joback Method
cpg	1758.80	J/mol×K	1315.06	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321881&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point