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

Inchi: InChI=1S/C30H59NO4/c1-6-8-10-11-12-13-14-15-16-17-18-19-20-21-22-23-25-34-29(32

InchiKey: MBNCOGWZCOUYRJ-UHFFFAOYSA-N

Formula: C30H59NO4

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

Mol. weight [g/mol]: 497.80

Physical Properties

Property code	Value	Unit	Source
hf	-1230.18	kJ/mol	Cheméo Relay (1.0)
hfus	75.00	kJ/mol	Joback Method
hvap	137.31	kJ/mol	Cheméo Relay (1.0)
log10ws	-7.89		Cheméo Relay (1.0)
logp	9.074		Crippen Method
mcvol	458.420	ml/mol	McGowan Method
rinpol	3514.00		NIST Webbook
rinpol	3514.00		NIST Webbook
tb	678.97	K	Cheméo Relay (1.0)
tf	291.19	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1651.20	J/mol×K	1049.94	Joback Method
cpg	1675.29	J/mol×K	1094.78	Joback Method
cpg	1696.85	J/mol×K	1139.63	Joback Method
cpg	1716.00	J/mol×K	1184.47	Joback Method
cpg	1732.89	J/mol×K	1229.31	Joback Method
cpg	1747.65	J/mol×K	1274.16	Joback Method
cpg	1760.41	J/mol×K	1319.00	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321895&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

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