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

Inchi: InChI=1S/C28H55NO4/c1-6-8-10-11-12-13-14-15-16-17-18-19-20-21-23-32-27(30)26(24

InchiKey: ZNQQEJNURQZRHO-UHFFFAOYSA-N

Formula: C28H55NO4

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

Mol. weight [g/mol]: 469.75

Physical Properties

Property code	Value	Unit	Source
hf	-1189.57	kJ/mol	Cheméo Relay (1.0)
hfus	69.82	kJ/mol	Joback Method
hvap	129.58	kJ/mol	Cheméo Relay (1.0)
log10ws	-7.27		Cheméo Relay (1.0)
logp	8.294		Crippen Method
mcvol	430.240	ml/mol	McGowan Method
rinpol	3089.00		NIST Webbook
rinpol	3089.00		NIST Webbook
tb	665.83	K	Cheméo Relay (1.0)
tf	284.67	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1520.48	J/mol×K	1004.18	Joback Method
cpg	1543.09	J/mol×K	1044.60	Joback Method
cpg	1563.61	J/mol×K	1085.01	Joback Method
cpg	1582.16	J/mol×K	1125.43	Joback Method
cpg	1598.80	J/mol×K	1165.84	Joback Method
cpg	1613.65	J/mol×K	1206.26	Joback Method
cpg	1626.78	J/mol×K	1246.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321893&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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

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