L-leucine, n-butoxycarbonyl-n-methyl-, pentadecyl ester

Inchi: InChI=1S/C27H53NO4/c1-6-8-10-11-12-13-14-15-16-17-18-19-20-22-31-26(29)25(23-24

InchiKey: HKERDHVMRIJCGO-UHFFFAOYSA-N

Formula: C27H53NO4

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

Mol. weight [g/mol]: 455.72

Physical Properties

Property code	Value	Unit	Source
hf	-1169.77	kJ/mol	Cheméo Relay (1.0)
hfus	67.24	kJ/mol	Joback Method
hvap	125.70	kJ/mol	Cheméo Relay (1.0)
log10ws	-6.95		Cheméo Relay (1.0)
logp	7.904		Crippen Method
mcvol	416.150	ml/mol	McGowan Method
rinpol	2929.00		NIST Webbook
rinpol	2929.00		NIST Webbook
tb	659.21	K	Cheméo Relay (1.0)
tf	280.66	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1455.55	J/mol×K	981.30	Joback Method
cpg	1477.49	J/mol×K	1019.88	Joback Method
cpg	1497.54	J/mol×K	1058.45	Joback Method
cpg	1515.78	J/mol×K	1097.03	Joback Method
cpg	1532.28	J/mol×K	1135.60	Joback Method
cpg	1547.11	J/mol×K	1174.18	Joback Method
cpg	1560.35	J/mol×K	1212.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321892&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