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

Inchi: InChI=1S/C24H47NO4/c1-7-8-9-10-11-12-13-14-15-16-17-28-23(26)22(18-20(2)3)25(6)2

InchiKey: XITXUJKARMVOAR-UHFFFAOYSA-N

Formula: C24H47NO4

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

Mol. weight [g/mol]: 413.64

Physical Properties

Property code	Value	Unit	Source
hf	-1127.63	kJ/mol	Cheméo Relay (1.0)
hfus	55.94	kJ/mol	Joback Method
hvap	110.77	kJ/mol	Cheméo Relay (1.0)
log10ws	-6.09		Cheméo Relay (1.0)
logp	6.590		Crippen Method
mcvol	373.880	ml/mol	McGowan Method
rinpol	2539.00		NIST Webbook
rinpol	2539.00		NIST Webbook
tb	639.77	K	Cheméo Relay (1.0)
tf	272.82	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1263.43	J/mol×K	912.22	Joback Method
cpg	1283.58	J/mol×K	946.44	Joback Method
cpg	1302.27	J/mol×K	980.67	Joback Method
cpg	1319.53	J/mol×K	1014.89	Joback Method
cpg	1335.42	J/mol×K	1049.12	Joback Method
cpg	1349.97	J/mol×K	1083.34	Joback Method
cpg	1363.24	J/mol×K	1117.57	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321876&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