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

Inchi: InChI=1S/C29H57NO4/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-33-28(31)27(2

InchiKey: PVKMCCGPFKKHPT-UHFFFAOYSA-N

Formula: C29H57NO4

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

Mol. weight [g/mol]: 483.78

Physical Properties

Property code	Value	Unit	Source
hf	-1226.24	kJ/mol	Cheméo Relay (1.0)
hfus	68.89	kJ/mol	Joback Method
hvap	130.61	kJ/mol	Cheméo Relay (1.0)
log10ws	-7.66		Cheméo Relay (1.0)
logp	8.540		Crippen Method
mcvol	444.330	ml/mol	McGowan Method
rinpol	3197.00		NIST Webbook
rinpol	3197.00		NIST Webbook
tb	673.94	K	Cheméo Relay (1.0)
tf	291.27	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1585.94	J/mol×K	1026.62	Joback Method
cpg	1608.93	J/mol×K	1068.63	Joback Method
cpg	1629.66	J/mol×K	1110.64	Joback Method
cpg	1648.23	J/mol×K	1152.64	Joback Method
cpg	1664.77	J/mol×K	1194.65	Joback Method
cpg	1679.36	J/mol×K	1236.66	Joback Method
cpg	1692.13	J/mol×K	1278.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321880&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