

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

Inchi: InChI=1S/C30H59NO4/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-34-29(32)24-25-26-27-28-30-31-33-34-35-36-37-38-39-40-41-42-43-44-45-46-47-48-49-50-51-52-53-54-55-56-57-58-59-60-61-62-63-64-65-66-67-68-69-70-71-72-73-74-75-76-77-78-79-80-81-82-83-84-85-86-87-88-89-90-91-92-93-94-95-96-97-98-99-100
InchiKey: AYKJWKHVOIPLMQ-UHFFFAOYSA-N
Formula: C30H59NO4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCC(C)C
Mol. weight [g/mol]: 497.80

Physical Properties

Property code	Value	Unit	Source
hf	-1246.22	kJ/mol	Cheméo Relay (1.0)
hfus	71.48	kJ/mol	Joback Method
hvap	134.49	kJ/mol	Cheméo Relay (1.0)
log10ws	-7.97		Cheméo Relay (1.0)
logp	8.930		Crippen Method
mcvol	458.420	ml/mol	McGowan Method
rinpol	3418.00		NIST Webbook
rinpol	3418.00		NIST Webbook
tb	680.52	K	Cheméo Relay (1.0)
tf	294.51	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1651.38	J/mol×K	1049.50	Joback Method
cpg	1675.08	J/mol×K	1093.76	Joback Method
cpg	1696.29	J/mol×K	1138.02	Joback Method
cpg	1715.14	J/mol×K	1182.28	Joback Method
cpg	1731.75	J/mol×K	1226.54	Joback Method
cpg	1746.26	J/mol×K	1270.80	Joback Method
cpg	1758.80	J/mol×K	1315.06	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U321881&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

Latest version available from:

<https://www.chemeo.com/cid/97-176-0/L-Leucine-N-isobutoxycarbonyl-N-methyl-octadecyl-ester.pdf>

Generated by Cheméo on 2026-07-21 23:01:35.392095102 +0000 UTC m=+185991.233980478.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.