

L-Leucine, N-neopentylloxycarbonyl-N-methyl-, pentadecyl ester

InChI: InChI=1S/C28H55NO4/c1-8-9-10-11-12-13-14-15-16-17-18-19-20-21-32-26(30)25(22-24)31
InChIKey: GAVPSZMEXLQUAX-UHFFFAOYSA-N

Formula: C28H55NO4
SMILES: CCCCCCCCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCC(C)(C)C
Mol. weight [g/mol]: 469.75

Physical Properties

Property code	Value	Unit	Source
hfus	62.41	kJ/mol	Joback Method
log10ws	-7.50		Cheméo Relay (1.0)
logp	8.150		Crippen Method
mcvol	430.240	ml/mol	McGowan Method
rinpol	2921.00		NIST Webbook
rinpol	2921.00		NIST Webbook
tb	663.10	K	Cheméo Relay (1.0)
tf	309.62	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1520.05	J/mol×K	1000.95	Joback Method
cpg	1542.17	J/mol×K	1040.17	Joback Method
cpg	1562.50	J/mol×K	1079.39	Joback Method
cpg	1581.13	J/mol×K	1118.61	Joback Method
cpg	1598.17	J/mol×K	1157.83	Joback Method
cpg	1613.74	J/mol×K	1197.06	Joback Method
cpg	1627.94	J/mol×K	1236.28	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U321916&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>

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion 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

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