

L-Leucine, N-benzyloxycarbonyl-N-methyl-, isobutyl ester

Inchi:	InChI=1S/C19H29NO4/c1-14(2)11-17(18(21)23-12-15(3)4)20(5)19(22)24-13-16-9-7-6-8-
InchiKey:	DGKZHIXHVKODBP-UHFFFAOYSA-N
Formula:	C19H29NO4
SMILES:	CC(C)COC(=O)C(CC(C)C)N(C)C(=O)OCc1ccccc1
Mol. weight [g/mol]:	335.44

Physical Properties

Property code	Value	Unit	Source
hfus	37.03	kJ/mol	Joback Method
hvap	95.03	kJ/mol	Cheméo Relay (1.0)
log10ws	-3.81		Cheméo Relay (1.0)
logp	3.869		Crippen Method
mcvol	279.670	ml/mol	McGowan Method
rinpol	2157.00		NIST Webbook
rinpol	2157.00		NIST Webbook
tb	618.93	K	Cheméo Relay (1.0)
tf	282.61	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	863.34	J/mol×K	824.50	Joback Method
cpg	879.82	J/mol×K	858.56	Joback Method
cpg	895.09	J/mol×K	892.63	Joback Method
cpg	909.19	J/mol×K	926.69	Joback Method
cpg	922.15	J/mol×K	960.75	Joback Method
cpg	934.00	J/mol×K	994.82	Joback Method
cpg	944.79	J/mol×K	1028.88	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U322036&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/ci990307I>

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

Legend

cpg:	Ideal gas heat capacity
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

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