

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

Inchi:	InChI=1S/C21H33NO4/c1-5-6-7-11-14-25-20(23)19(15-17(2)3)22(4)21(24)26-16-18-12-9
InchiKey:	DIWVROZPZOBSPP-UHFFFAOYSA-N
Formula:	C21H33NO4
SMILES:	CCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCc1ccccc1
Mol. weight [g/mol]:	363.50

Physical Properties

Property code	Value	Unit	Source
hfus	45.74	kJ/mol	Joback Method
log10ws	-4.52		Cheméo Relay (1.0)
logp	4.793		Crippen Method
mcvol	307.850	ml/mol	McGowan Method
pc	1278.25	kPa	Joback Method
rinpol	2388.00		NIST Webbook
rinpol	2388.00		NIST Webbook
tb	635.78	K	Cheméo Relay (1.0)
tf	270.90	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	981.52	J/mol×K	870.70	Joback Method
cpg	998.14	J/mol×K	904.62	Joback Method
cpg	1013.53	J/mol×K	938.54	Joback Method
cpg	1027.70	J/mol×K	972.47	Joback Method
cpg	1040.72	J/mol×K	1006.39	Joback Method
cpg	1052.62	J/mol×K	1040.31	Joback Method
cpg	1063.43	J/mol×K	1074.23	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U322040&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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