L-Leucine, N-allyloxycarbonyl-N-methyl-, nonyl ester

Inchi: InChI=1S/C20H37NO4/c1-6-8-9-10-11-12-13-15-24-19(22)18(16-17(3)4)21(5)20(23)25-1

InchiKey: XGZRBEDPZINOIA-UHFFFAOYSA-N

Formula: C20H37NO4

SMILES: C=CCOC(=O)N(C)C(CC(C)C)C(=O)OCCCCCCCCC

Mol. weight [g/mol]: 355.52

Physical Properties

Property code	Value	Unit	Source
hfus	47.82	kJ/mol	Joback Method
log10ws	-4.66		Cheméo Relay (1.0)
logp	4.949		Crippen Method
mcvol	313.220	ml/mol	McGowan Method
rinpol	2192.00		NIST Webbook
tb	629.02	K	Cheméo Relay (1.0)
tf	255.56	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	986.33	J/mol×K	817.82	Joback Method
cpg	1004.33	J/mol×K	848.98	Joback Method
cpg	1021.26	J/mol×K	880.14	Joback Method
cpg	1037.13	J/mol×K	911.30	Joback Method
cpg	1051.97	J/mol×K	942.46	Joback Method
cpg	1065.82	J/mol×K	973.62	Joback Method
cpg	1078.69	J/mol×K	1004.78	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U321902&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
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