

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

Inchi: InChI=1S/C20H39NO4/c1-6-8-9-10-11-12-13-15-24-19(22)18(16-17(3)4)21(5)20(23)25-1

InchiKey: ILLCTVFGWJWSAW-UHFFFAOYSA-N

Formula: C20H39NO4

SMILES: CCCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCCC

Mol. weight [g/mol]: 357.53

Physical Properties

Property code	Value	Unit	Source
hf	-1030.52	kJ/mol	Cheméo Relay (1.0)
hfus	49.10	kJ/mol	Joback Method
hvap	96.81	kJ/mol	Cheméo Relay (1.0)
log10ws	-4.82		Cheméo Relay (1.0)
logp	5.173		Crippen Method
mcvol	317.520	ml/mol	McGowan Method
rinpol	2197.00		NIST Webbook
rinpol	2197.00		NIST Webbook
tb	613.35	K	Cheméo Relay (1.0)
tf	256.89	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1013.53	J/mol×K	821.14	Joback Method
cpg	1032.07	J/mol×K	852.25	Joback Method
cpg	1049.49	J/mol×K	883.35	Joback Method
cpg	1065.82	J/mol×K	914.46	Joback Method
cpg	1081.08	J/mol×K	945.57	Joback Method
cpg	1095.30	J/mol×K	976.68	Joback Method
cpg	1108.50	J/mol×K	1007.78	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U321859&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):

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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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