

L-Leucine, methyl ester

Other names:	Leucine, methyl ester, L- (+)-L-Leucine methyl ester Leucine methyl ester Methyl L-leucinate Leu, propyl ester (d) leucine methyl ester
Inchi:	InChI=1S/C7H15NO2/c1-5(2)4-6(8)7(9)10-3/h5-6H,4,8H2,1-3H3/t6-/m1/s1
InchiKey:	QVDXUKJJGUSGLS-ZCFIWIBFSA-N
Formula:	C7H15NO2
SMILES:	<chem>COC(=O)C(N)CC(C)C</chem>
Mol. weight [g/mol]:	145.20
CAS:	2666-93-5

Physical Properties

Property code	Value	Unit	Source
gf	-164.29	kJ/mol	Joback Method
hf	-409.38	kJ/mol	Joback Method
hfus	14.82	kJ/mol	Joback Method
hvap	50.20	kJ/mol	Joback Method
log10ws	-0.92		Crippen Method
logp	0.533		Crippen Method
mcvol	126.910	ml/mol	McGowan Method
pc	3188.33	kPa	Joback Method
rinpol	1260.00		NIST Webbook
rinpol	1261.00		NIST Webbook
rinpol	1262.00		NIST Webbook
rinpol	1267.00		NIST Webbook
rinpol	1269.00		NIST Webbook
tb	507.50	K	Joback Method
tc	703.81	K	Joback Method
tf	294.07	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	294.09	J/mol×K	507.50	Joback Method
cpg	306.40	J/mol×K	540.22	Joback Method
cpg	318.17	J/mol×K	572.94	Joback Method
cpg	329.42	J/mol×K	605.65	Joback Method
cpg	340.15	J/mol×K	638.37	Joback Method
cpg	350.36	J/mol×K	671.09	Joback Method
cpg	360.05	J/mol×K	703.81	Joback Method
hvapt	39.40	kJ/mol	336.50	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2666935&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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