Leucine

Other names:	L-Leucine Leucine, L- L-«alpha»-Aminoisocaproic acid «alpha»-Amino-«gamma»-methylvaleric acid (S)-(+)-Leucine L-(+)-Leucine Leu Pentanoic acid, 2-amino-4-methyl-, (S)- 2-Amino-4-methylpentanoic acid, (L)- 2-Amino-4-methylvaleric acid, (L)- iso-C4H9CH(NH2)COOH L-(-)-2-Amino-4-methylpentanoic acid Norvaline, 4-methyl-, (L)- Valeric acid, 2-amino-4-methyl-, (S)- Leucin (S)-2-Amino-4-methylpentanoic acid (S)-Leucine (S)-2-Amino-4-methylvaleric acid L-Norvaline, 4-methyl- NSC 46709
Inchi:	InChI=1S/C6H13NO2/c1-4(2)3-5(7)6(8)9/h4-5H,3,7H2,1-2H3,(H,8,9)/t5-/m1/s1
InchiKey:	ROHFNLRQFUQHCH-RXMQYKEDSA-N
Formula:	C6H13NO2
SMILES:	CC(C)CC(N)C(=O)O
Mol. weight [g/mol]:	131.17
CAS:	61-90-5

Physical Properties

Property code	Value	Unit	Source
affp	914.60	kJ/mol	NIST Webbook
basg	880.60	kJ/mol	NIST Webbook
chg	-3570.00 ± 1.90	kJ/mol	NIST Webbook
chs	-3600.40	kJ/mol	NIST Webbook
chs	-3596.00	kJ/mol	NIST Webbook
chs	-3581.50 ± 0.84	kJ/mol	NIST Webbook
chs	-3572.00 ± 0.30	kJ/mol	NIST Webbook
gf	-204.53	kJ/mol	Joback Method

hf	-408.75	kJ/mol	Joback Method
hfl	-648.90 ± 2.00	kJ/mol	NIST Webbook
hfs	-646.80	kJ/mol	NIST Webbook
hfs	-637.39 ± 0.92	kJ/mol	NIST Webbook
hfus	15.13	kJ/mol	Joback Method
hvap	62.24	kJ/mol	Joback Method
ie	8.51	eV	NIST Webbook
log10ws	-0.74		Crippen Method
logp	0.444		Crippen Method
mcvol	112.820	ml/mol	McGowan Method
pc	4077.71	kPa	Joback Method
ss	211.79	J/mol×K	NIST Webbook
tb	554.38	K	Joback Method
tc	743.19	K	Joback Method
tf	321.39	K	Joback Method
vc	0.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.64	J/mol×K	680.26	Joback Method
cpg	326.94	J/mol×K	743.19	Joback Method
cpg	319.50	J/mol×K	711.72	Joback Method
cpg	275.71	J/mol×K	554.38	Joback Method
cpg	285.39	J/mol×K	585.85	Joback Method
cpg	294.59	J/mol×K	617.32	Joback Method
cpg	303.34	J/mol×K	648.79	Joback Method
cps	200.96	J/mol×K	298.15	NIST Webbook
cps	190.60	J/mol×K	298.00	NIST Webbook
cps	201.40	J/mol×K	298.15	NIST Webbook
cps	191.00	J/mol×K	298.00	NIST Webbook
hsubt	150.60 ± 0.80	kJ/mol	455.00	NIST Webbook
hsubt	151.00 ± 0.80	kJ/mol	455.00	NIST Webbook
hsubt	148.70 ± 6.50	kJ/mol	459.00	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=C61905&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
chg:	Standard gas enthalpy of combustion
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:
https://www.chemeo.com/cid/15-216-5/Leucine.pdf
Generated by Cheméo on 2024-04-19 21:19:05.789716456 +0000 UTC m=+15850794.710293768.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.