N-Acetyl-L-leucine

Other names:	2-acetamido-4-methylpentanoic acid
	Acetyl-L-leucine
	L-Leucine, N-acetyl-
	Leucine, N-acetyl-, L-
	N-Acetylleucine
Inchi:	InChI=1S/C8H15NO3/c1-5(2)4-7(8(11)12)9-6(3)10/h5,7H,4H2,1-3H3,(H,9,10)(H,11,12)
InchiKey:	WXNXCEHXYPACJF-UHFFFAOYSA-N
Formula:	C8H15NO3
SMILES:	CC(=O)NC(CC(C)C)C(=O)O
Mol. weight [g/mol]:	173.21
CAS:	1188-21-2

Physical Properties

Property code	Value	Unit	Source
gf	-293.67	kJ/mol	Joback Method
hf	-542.93	kJ/mol	Joback Method
hfus	21.82	kJ/mol	Joback Method
hvap	69.23	kJ/mol	Joback Method
log10ws	-1.13		Aqueous Solubility Prediction Method
logp	0.622		Crippen Method
mcvol	142.570	ml/mol	McGowan Method
pc	3306.75	kPa	Joback Method
tb	631.65	K	Joback Method
tc	816.96	K	Joback Method
tf	363.26	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.42	J/mol×K	631.65	Joback Method
cpg	383.99	J/mol×K	662.54	Joback Method
cpg	394.01	J/mol×K	693.42	Joback Method

cpg	403.50	J/mol×K	724.31	Joback Method
cpg	412.46	J/mol×K	755.19	Joback Method
cpg	420.91	J/mol×K	786.08	Joback Method
cpg	428.87	J/mol×K	816.96	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1188212&Units=SI

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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume