6-Aminohexanoic acid

Other names: 6-aminocaproic acid
Inchi: InChI=1S/C6H13NO2/c7-5-3-1-2-4-6(8)9/h1-5,7H2,(H,8,9)
InchiKey: SLXKOJJOQWFEFD-UHFFFAOYSA-N
Formula: C6H13NO2
SMILES: NCCCCCC(=O)O
Mol. weight [g/mol]: 131.17

Physical Properties

Property code	Value	Unit	Source
gf	-199.65	kJ/mol	Joback Method
hf	-398.19	kJ/mol	Joback Method
hfus	22.18	kJ/mol	Joback Method
hvap	63.02	kJ/mol	Joback Method
log10ws	-0.87		Crippen Method
logp	0.590		Crippen Method
mcvol	112.820	ml/mol	McGowan Method
pc	3995.65	kPa	Joback Method
tb	555.26	K	Joback Method
tc	736.90	K	Joback Method
tf	351.39	K	Joback Method
vc	0.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.92	J/mol×K	555.26	Joback Method
cpg	284.12	J/mol×K	585.53	Joback Method
cpg	292.90	J/mol×K	615.81	Joback Method
cpg	301.26	J/mol×K	646.08	Joback Method
cpg	309.22	J/mol×K	676.36	Joback Method
cpg	316.80	J/mol×K	706.63	Joback Method
cpg	324.00	J/mol×K	736.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Measurement and Correlation of the Solubility of Aminocaproic Acid in Some Pure and Binary Solvents:	https://www.doi.org/10.1021/acs.jced.9b00543
Binary Diffusion Coefficients of Aqueous Straight-Chain Amino Acids at Infinite-Dilution Concentration and Temperatures from (298.2 to 333.2) K:	https://www.doi.org/10.1021/je301370s
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Osmotic and activity coefficients of alpha, omega-amino acids in aqueous solutions at 298.15 K:	https://www.doi.org/10.1016/j.fluid.2014.02.004
Effect of temperature on the dilution enthalpies of alpha,omega-amino acids in aqueous solutions:	https://www.doi.org/10.1016/j.jct.2011.04.019
Volumetric Properties of Some a,w-Aminocarboxylic Acids in Aqueous Solutions at T = (298.15 to 318.15) K:	https://www.doi.org/10.1021/je100476h
Partial Molar Volumes, Partial Molar Compressibilities, and Viscosities of Glycine, Sodium Acetate, and Magnesium Acetate in Water and in Aqueous Solutions of Sodium Chloride over a Temperature Range of 293.2-333.2 K:	https://www.doi.org/10.1021/acs.jced.8b00236
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6001903&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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