

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:	NCCCCC(=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
mvol	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/molxK	555.26	Joback Method
cpg	284.12	J/molxK	585.53	Joback Method
cpg	292.90	J/molxK	615.81	Joback Method
cpg	301.26	J/molxK	646.08	Joback Method
cpg	309.22	J/molxK	676.36	Joback Method
cpg	316.80	J/molxK	706.63	Joback Method
cpg	324.00	J/molxK	736.90	Joback Method

Sources

Binary Diffusion Coefficients of Aqueous Straight-Chain Amino Acids at Various Concentration and Temperatures from (298.2 to 333.2) K: McGowan Method:

<https://www.doi.org/10.1021/je301370s>

Volumetric Properties of Some α,ω -Aminocarboxylic Acids in Aqueous Sodium Acetate and Magnesium Acetate Solutions at T = (288.15 to 318.15) K:

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

<http://link.springer.com/article/10.1007/BF02311772>

<https://www.doi.org/10.1021/je100476h>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=B6001903&Units=SI>

Osmotic and activity coefficients of α,ω -amino acids in aqueous solution. Partial molar compressibilities, and viscosities of aqueous amino acid solutions. The solubility of amino acids in sodium chloride and potassium chloride solutions. The effect of temperature on the partition enthalpies of α,ω -amino acids in aqueous solutions:

https://www.chemeo.com/doc/models/crippen_log10ws

<https://www.doi.org/10.1016/j.fluid.2014.02.004>

<https://www.doi.org/10.1021/acs.jced.8b00236>

<https://www.doi.org/10.1021/acs.jced.9b00543>

<https://www.doi.org/10.1016/j.jct.2011.04.019>

<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

Latest version available from:

<https://www.chemeo.com/cid/98-502-6/6-Aminohexanoic-acid.pdf>

Generated by Cheméo on 2024-04-23 15:06:26.343133293 +0000 UTC m=+16174035.263710614.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.