5-Aminovaleric acid

Other names:	5-Aminopentanoic acid H2N(CH2)4COOH Pentanoic acid, 5-amino- Valeric acid, 5-amino- «delta»-Amino-n-valeric acid «delta»-Aminovaleric acid Â«deltaÂ»-Amino-n-valeric acid Â«deltaÂ»-Aminovaleric acid
Inchi:	InChI=1S/C5H11NO2/c6-4-2-1-3-5(7)8/h1-4,6H2,(H,7,8)
InchiKey:	JJMDCOVWQOJGCB-UHFFFAOYSA-N
Formula:	C5H11NO2
SMILES:	NCCCCC(=O)O
Mol. weight [g/mol]:	117.15
CAS:	660-88-8

Physical Properties

Property code	Value	Unit	Source
chs	-2935.49 ± 0.42	kJ/mol	NIST Webbook
chs	-2935.50 ± 0.84	kJ/mol	NIST Webbook
gf	-208.07	kJ/mol	Joback Method
hf	-460.20 ± 3.00	kJ/mol	NIST Webbook
hfs	-604.17 ± 0.42	kJ/mol	NIST Webbook
hfus	19.59	kJ/mol	Joback Method
hsub	144.00 ± 3.00	kJ/mol	NIST Webbook
hvap	60.79	kJ/mol	Joback Method
ie	9.40	eV	NIST Webbook
log10ws	-0.45		Crippen Method
logp	0.200		Crippen Method
mcvol	98.730	ml/mol	McGowan Method
pc	4528.58	kPa	Joback Method
tb	532.38	K	Joback Method
tc	715.91	K	Joback Method
tf	340.12	K	Joback Method
vc	0.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.15	J/mol×K	624.15	Joback Method
cpg	262.27	J/mol×K	654.74	Joback Method
cpg	269.03	J/mol×K	685.33	Joback Method
cpg	231.63	J/mol×K	532.38	Joback Method
cpg	239.85	J/mol×K	562.97	Joback Method
cpg	247.69	J/mol×K	593.56	Joback Method
cpg	275.46	J/mol×K	715.91	Joback Method
cps	163.70	J/mol×K	298.00	NIST Webbook
hsubt	141.80 ± 0.50	kJ/mol	389.00	NIST Webbook
hsubt	144.00 ± 3.00	kJ/mol	289.00	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C660888&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Binary Diffusion Coefficients of Aqueous Straight-Chain Amino Acids at Infinitesimal Concentration and Temperatures from (298.2 to 333.2) K:	https://www.doi.org/10.1021/je301370s
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
Partial Molar Volumes, Partial Molar Compressibilities, and Viscosities of alpha,w-Amino Acids in Water and in Aqueous Solutions of Sodium Chloride over a Temperature Range of 193.2-333.2 K:	https://www.doi.org/10.1021/acs.jced.8b00236

Legend

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
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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