Aminocaproic acid

Other names:

177 J.D.
6-Amino-n-hexanoic acid
6-Aminocaproic acid
6-Aminohexanoic acid
ACS
Acepramin
Acepramine
Afibrin
Amicar
Amikar
Aminokapron
Atsemin
CL 10304
CY 116
Caplamin
Capracid
Capramol
Capranol
Caprocid
Caprolisin
EACA
EACS
Epsamon
Epsicapron
Epsikapron
Epsilcapramin
Hemocaprol
Hemopar
Hepin
Hexanoic acid, 6-amino-
Ipsilon
NSC-26154
Respramin
«epsilon»-Amino-n-caproic acid
«epsilon»-Amino-n-hexanoic acid
«epsilon»-Aminocaproic acid
«epsilon»-Aminohexanoic acid
«epsilon»-Norleucine
«omega»-Aminocaproic acid
«omega»-Aminohexanoic acid

Â«epsilonÂ»-Amino-n-caproic acid
Â«epsilonÂ»-Amino-n-hexanoic acid
Â«epsilonÂ»-Aminocaproic acid
Â«epsilonÂ»-Aminohexanoic acid
Â«epsilonÂ»-Norleucine
Â«omegaÂ»-Aminocaproic acid
Â«omegaÂ»-Aminohexanoic 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
CAS: 60-32-2

Physical Properties

Property code	Value	Unit	Source
chs	-3581.61 ± 0.25	kJ/mol	NIST Webbook
chs	-3579.80 ± 1.30	kJ/mol	NIST Webbook
gf	-199.65	kJ/mol	Joback Method
hf	-482.40 ± 3.00	kJ/mol	NIST Webbook
hfs	-637.35 ± 0.48	kJ/mol	NIST Webbook
hfus	22.18	kJ/mol	Joback Method
hsub	155.00 ± 3.00	kJ/mol	NIST Webbook
hsub	155.00 ± 3.00	kJ/mol	NIST Webbook
hvap	63.02	kJ/mol	Joback Method
log10ws	-0.97		Aqueous Solubility Prediction 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	479.65	K	Aqueous Solubility Prediction Method
vc	0.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	309.22	J/mol×K	676.36	Joback Method
cpg	316.80	J/mol×K	706.63	Joback Method
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	324.00	J/mol×K	736.90	Joback Method
cps	175.60	J/mol×K	298.00	NIST Webbook
hsubt	153.30 ± 0.80	kJ/mol	397.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C60322&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

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
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