5-Aminohexanoic acid

Other names: 5-Aminocaproic acid
Inchi: InChI=1S/C6H13NO2/c1-5(7)3-2-4-6(8)9/h5H,2-4,7H2,1H3,(H,8,9)
InchiKey: IPCUHQYGWOKSLR-UHFFFAOYSA-N
Formula: C6H13NO2
SMILES: CC(N)CCCC(=O)O
Mol. weight [g/mol]: 131.17
CAS: 628-47-7

Physical Properties

Property code	Value	Unit	Source
gf	-202.09	kJ/mol	Joback Method
hf	-403.47	kJ/mol	Joback Method
hfus	18.66	kJ/mol	Joback Method
hvap	62.63	kJ/mol	Joback Method
log10ws	-0.98		Crippen Method
logp	0.588		Crippen Method
mcvol	112.820	ml/mol	McGowan Method
pc	4036.37	kPa	Joback Method
tb	554.82	K	Joback Method
tc	739.98	K	Joback Method
tf	336.39	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.32	J/mol×K	554.82	Joback Method
cpg	284.75	J/mol×K	585.68	Joback Method
cpg	293.74	J/mol×K	616.54	Joback Method
cpg	302.29	J/mol×K	647.40	Joback Method
cpg	310.42	J/mol×K	678.26	Joback Method
cpg	318.14	J/mol×K	709.12	Joback Method
cpg	325.46	J/mol×K	739.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C628477&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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