

5-AMINOCAPROIC 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

Physical Properties

Property code	Value	Unit	Source
chs	-3575.60 ± 1.30	kJ/mol	NIST Webbook
gf	-202.09	kJ/mol	Joback Method
hf	-507.44	kJ/mol	Cheméo Relay (1.0)
hfus	18.66	kJ/mol	Joback Method
hvap	79.27	kJ/mol	Cheméo Relay (1.0)
ie	8.79	eV	Cheméo Relay (1.0)
log10ws	0.12		Cheméo Relay (1.0)
logp	0.588		Crippen Method
mcvol	112.820	ml/mol	McGowan Method
pc	4036.37	kPa	Joback Method
tb	514.93	K	Cheméo Relay (1.0)
tc	692.52	K	Cheméo Relay (1.0)
tf	377.89	K	Cheméo Relay (1.0)
vc	0.397	m3/kmol	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C628477&Units=SI>

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

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

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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

Legend

chs:	Standard solid enthalpy of combustion
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
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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