Guanidine

Other names:	(NH2)2C=NH
	Aminoformamidine
	Aminomethanamidine
	Carbamamidine
	Carbamidine
	Guanidin
	Imidourea
	Iminourea
Inchi:	InChI=1S/CH5N3/c2-1(3)4/h(H5,2,3,4)
InchiKey:	ZRALSGWEFCBTJO-UHFFFAOYSA-N
Formula:	CH5N3
SMILES:	N=C(N)N
Mol. weight [g/mol]:	59.07
CAS:	113-00-8

Physical Properties

Property code	Value	Unit	Source
affp	986.30	kJ/mol	NIST Webbook
basg	949.40	kJ/mol	NIST Webbook
chs	-1052.10 ± 1.00	kJ/mol	NIST Webbook
gf	294.04	kJ/mol	Joback Method
hf	201.94	kJ/mol	Joback Method
hfs	-56.00 ± 1.00	kJ/mol	NIST Webbook
hvap	51.18	kJ/mol	Joback Method
ie	9.10 ± 0.05	eV	NIST Webbook
log10ws	-1.02		Crippen Method
logp	-1.161		Crippen Method
mcvol	50.590	ml/mol	McGowan Method
tb	451.68	K	Joback Method
tf	414.15	K	Determination and prediction of solubilities of active pharmaceutical ingredients in selected organic solvents

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	100.28	J/mol×K	451.68	Joback Method
cpg	24.30	J/mol×K	100.12	Joback Method
cpg	24.30	J/mol×K	100.12	Joback Method
cpg	24.30	J/mol×K	100.12	Joback Method
cpg	24.30	J/mol×K	100.12	Joback Method
cpg	24.30	J/mol×K	100.12	Joback Method
cpg	24.30	J/mol×K	100.12	Joback Method

Sources

Determination and prediction of solubilities of active pharmaceutical ingredients in selected organic solvents:	https://www.doi.org/10.1016/j.fluid.2015.07.032
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C113008&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
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
hfs:	Solid phase enthalpy of formation 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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point