Aminoacetonitrile

Other names:	H2NCH2CN
	Acetonitrile, amino-
	AAN
	«alpha»-Aminoacetonitrile
	2-Aminoacetonitrile
	Cyanomethylamine
	Glycinenitrile
	Glycinonitrile
	NCCH2NH2
Inchi:	InChI=1S/C2H4N2/c3-1-2-4/h1,3H2
InchiKey:	DFNYGALUNNFWKJ-UHFFFAOYSA-N
Formula:	C2H4N2
SMILES:	N#CCN
Mol. weight [g/mol]:	56.07
CAS:	540-61-4

Physical Properties

Property code	Value	Unit	Source
affp	824.90	kJ/mol	NIST Webbook
basg	791.00	kJ/mol	NIST Webbook
gf	165.59	kJ/mol	Joback Method
hf	114.06	kJ/mol	Joback Method
hfus	7.64	kJ/mol	Joback Method
hvap	41.17	kJ/mol	Joback Method
log10ws	0.04		Crippen Method
logp	-0.531		Crippen Method
mcvol	50.400	ml/mol	McGowan Method
pc	5266.25	kPa	Joback Method
tb	419.77	K	Joback Method
tc	631.29	K	Joback Method
tf	260.55	K	Joback Method
vc	0.203	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	88.64	J/mol×K	419.77	Joback Method
cpg	92.71	J/mol×K	455.02	Joback Method
cpg	96.59	J/mol×K	490.28	Joback Method
cpg	100.29	J/mol×K	525.53	Joback Method
cpg	103.81	J/mol×K	560.78	Joback Method
cpg	107.17	J/mol×K	596.04	Joback Method
cpg	110.36	J/mol×K	631.29	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	331.20	K	2.00	NIST Webbook
tbrp	331.00	K	2.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C540614&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

affp: Proton affinity
basg: Gas basicity
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume