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

Physical Properties

Property code	Value	Unit	Source
affp	824.90	kJ/mol	NIST Webbook
basg	791.00	kJ/mol	NIST Webbook
hf	136.93	kJ/mol	Cheméo Relay (1.0)
hfus	7.64	kJ/mol	Joback Method
ie	10.06	eV	Cheméo Relay (1.0)
logp	-0.531		Crippen Method
mcvol	50.400	ml/mol	McGowan Method
tb	456.20	K	Cheméo Relay (1.0)
tf	280.86	K	Cheméo Relay (1.0)

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

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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C540614&Units=SI

Legend

affp: Proton affinity
basg: Gas basicity
cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tf: Normal melting (fusion) point

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