Benzonitrile, m-amino-

Other names:	m-Aminobenzonitrile
	m-Cyanoaniline
	3-Aminobenzonitrile
	3-Cyanoaniline
	m-Anthranilonitrile
	Benzonitrile, 3-amino-
Inchi:	InChI=1S/C7H6N2/c8-5-6-2-1-3-7(9)4-6/h1-4H,9H2
InchiKey:	NJXPYZHXZZCTNI-UHFFFAOYSA-N
Formula:	C7H6N2
SMILES:	N#Cc1cccc(N)c1
Mol. weight [g/mol]:	118.14
CAS:	2237-30-1

Physical Properties

Property code	Value	Unit	Source
affp	842.30	kJ/mol	NIST Webbook
basg	810.40	kJ/mol	NIST Webbook
gf	310.47	kJ/mol	Joback Method
hf	235.92	kJ/mol	Joback Method
hfus	14.24	kJ/mol	Joback Method
hvap	55.23	kJ/mol	Joback Method
ie	8.61 ± 0.05	eV	NIST Webbook
log10ws	-1.46		Crippen Method
logp	1.140		Crippen Method
mcvol	97.090	ml/mol	McGowan Method
pc	4205.63	kPa	Joback Method
tb	562.00 ± 1.00	K	NIST Webbook
tb	562.20	K	NIST Webbook
tc	812.67	K	Joback Method
tf	326.65 ± 2.00	K	NIST Webbook
tf	326.50 ± 0.50	K	NIST Webbook
vc	0.374	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.89	J/mol×K	565.83	Joback Method
cpg	214.76	J/mol×K	606.97	Joback Method
cpg	222.99	J/mol×K	648.11	Joback Method
cpg	230.59	J/mol×K	689.25	Joback Method
cpg	237.61	J/mol×K	730.39	Joback Method
cpg	244.08	J/mol×K	771.53	Joback Method
cpg	250.02	J/mol×K	812.67	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C2237301&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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