

Benzonitrile, 4-amino-

Other names:	Benzonitrile, p-amino- p-Aminobenzonitrile p-Cyanoaniline 1-Amino-4-cyanobenzene 4-Aminobenzonitrile 4-Cyanoaniline Aniline, p-cyano-
Inchi:	InChI=1S/C7H6N2/c8-5-6-1-3-7(9)4-2-6/h1-4H,9H2
InchiKey:	YBAZINRZQSAIAY-UHFFFAOYSA-N
Formula:	C7H6N2
SMILES:	N#Cc1ccc(N)cc1
Mol. weight [g/mol]:	118.14
CAS:	873-74-5

Physical Properties

Property code	Value	Unit	Source
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	8.17	eV	NIST Webbook
ie	8.51	eV	NIST Webbook
ie	8.64 ± 0.04	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	565.83	K	Joback Method
tc	812.67	K	Joback Method
tf	359.40 ± 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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C873745&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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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