Benzonitrile, 4-(dimethylamino)-

Other names:	Benzonitrile, p-(dimethylamino)-
	p-(Dimethylamino)benzoic acid nitrile
	p-(Dimethylamino)benzonitrile
	p-(N,N-Dimethylamino)benzonitrile
	p-Cyano-N,N-dimethylaniline
	N,N-Dimethyl-p-cyanoaniline
	N,N-Dimethyl-4-cyanoaniline
	para(Dimethylamino)benzonitrile
	4-(Dimethylamino)benzenecarbonitrile
	4-(Dimethylamino)benzonitrile
	4-Cyano-N,N-dimethylaniline
	1-(Dimethylamino)-4-cyanobenzene
	NSC 409122
Inchi:	InChI=1S/C9H10N2/c1-11(2)9-5-3-8(7-10)4-6-9/h3-6H,1-2H3
InchiKey:	JYMNQRQQBJIMCV-UHFFFAOYSA-N
Formula:	C9H10N2
SMILES:	CN(C)c1ccc(C#N)cc1
Mol. weight [g/mol]:	146.19
CAS:	1197-19-9

Physical Properties

Property code	Value	Unit	Source
affp	889.10	kJ/mol	NIST Webbook
basg	862.60	kJ/mol	NIST Webbook
gf	371.64	kJ/mol	Joback Method
hf	228.38	kJ/mol	Joback Method
hfus	17.25	kJ/mol	Joback Method
hvap	51.09	kJ/mol	Joback Method
ie	7.99 ± 0.04	eV	NIST Webbook
ie	7.60	eV	NIST Webbook
ie	7.91	eV	NIST Webbook
log10ws	-1.73		Crippen Method
logp	1.624		Crippen Method
mcvol	125.270	ml/mol	McGowan Method
pc	3110.57	kPa	Joback Method
tb	591.20	K	NIST Webbook
tb	591.00	K	NIST Webbook

tc	776.47	K	Joback Method
tf	349.00	K	NIST Webbook
vc	0.475	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.92	J/mol×K	551.50	Joback Method
cpg	288.92	J/mol×K	588.99	Joback Method
cpg	300.13	J/mol×K	626.49	Joback Method
cpg	310.57	J/mol×K	663.98	Joback Method
cpg	320.28	J/mol×K	701.48	Joback Method
cpg	329.31	J/mol×K	738.97	Joback Method
cpg	337.70	J/mol×K	776.47	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1197199&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
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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