Benzonitrile, 4-acetyl-

Other names:	Benzonitrile, p-acetyl-
	p-Cyanoacetophenone
	Paracyanoacetophenone
	4-Acetylbenzonitrile
	4-Cyanoacetophenone
	4'-Cyanoacetophenone
	p-Acetylbenzonitrile
	4-Cyanophenyl methyl ketone
Inchi:	InChI=1S/C9H7NO/c1-7(11)9-4-2-8(6-10)3-5-9/h2-5H,1H3
InchiKey:	NLPHXWGWBKZSJC-UHFFFAOYSA-N
Formula:	C9H7NO
SMILES:	CC(=O)c1ccc(C#N)cc1
Mol. weight [g/mol]:	145.16
CAS:	1443-80-7

Physical Properties

Property code	Value	Unit	Source
affp	826.80	kJ/mol	NIST Webbook
basg	795.00	kJ/mol	NIST Webbook
ea	1.13 ± 0.10	eV	NIST Webbook
gf	131.94	kJ/mol	Joback Method
hf	48.27	kJ/mol	Joback Method
hfus	15.82	kJ/mol	Joback Method
hvap	55.79	kJ/mol	Joback Method
ie	9.78	eV	NIST Webbook
ie	9.82	eV	NIST Webbook
log10ws	-2.48		Crippen Method
logp	1.761		Crippen Method
mcvol	116.860	ml/mol	McGowan Method
pc	3348.98	kPa	Joback Method
tb	592.93	K	Joback Method
tc	829.52	K	Joback Method
tf	345.05	K	Joback Method
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.59	J/mol×K	592.93	Joback Method
cpg	264.55	J/mol×K	632.36	Joback Method
cpg	273.81	J/mol×K	671.79	Joback Method
cpg	282.40	J/mol×K	711.22	Joback Method
cpg	290.34	J/mol×K	750.65	Joback Method
cpg	297.67	J/mol×K	790.09	Joback Method
cpg	304.42	J/mol×K	829.52	Joback Method

Sources

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=C1443807&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
ea:	Electron affinity
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