Benzonitrile, 3-hydroxy-

Other names:	Benzonitrile, m-hydroxy-
	m-Cyanophenol
	m-Hydroxybenzonitrile
	3-Cyanophenol
	3-Hydroxybenzonitrile
	3-Hydroxybenzoic acid nitrile
Inchi:	InChI=1S/C7H5NO/c8-5-6-2-1-3-7(9)4-6/h1-4,9H
InchiKey:	SGHBRHKBCLLVCI-UHFFFAOYSA-N
Formula:	C7H5NO
SMILES:	N#Cc1cccc(O)c1
Mol. weight [g/mol]:	119.12
CAS:	873-62-1

Physical Properties

Property code	Value	Unit	Source
gf	99.03	kJ/mol	Joback Method
hf	36.29	kJ/mol	Joback Method
hfus	15.22	kJ/mol	Joback Method
hvap	56.94	kJ/mol	Joback Method
ie	9.39 ± 0.05	eV	NIST Webbook
log10ws	-1.37		Crippen Method
logp	1.264		Crippen Method
mcvol	92.980	ml/mol	McGowan Method
pc	4856.20	kPa	Joback Method
tb	568.94	K	Joback Method
tc	817.38	K	Joback Method
tf	371.78	K	Joback Method
vc	0.311	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	199.90	J/mol×K	568.94	Joback Method
cpg	207.76	J/mol×K	610.35	Joback Method

cpg	214.93	J/mol×K	651.75	Joback Method
cpg	221.50	J/mol×K	693.16	Joback Method
cpg	227.57	J/mol×K	734.57	Joback Method
cpg	233.22	J/mol×K	775.98	Joback Method
cpg	238.57	J/mol×K	817.38	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=C873621&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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