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

Physical Properties

Property code	Value	Unit	Source
af	0.5341		Cheméo Relay (1.0)
gf	99.03	kJ/mol	Joback Method
hf	48.07	kJ/mol	Cheméo Relay (1.0)
hfus	15.22	kJ/mol	Joback Method
hvap	76.12	kJ/mol	Cheméo Relay (1.0)
ie	9.39 ± 0.05	eV	NIST Webbook
log10ws	-0.76		Cheméo Relay (1.0)
logp	1.264		Crippen Method
mcvol	92.980	ml/mol	McGowan Method
pc	4856.20	kPa	Joback Method
tb	536.95	K	Cheméo Relay (1.0)
tc	797.33	K	Cheméo Relay (1.0)
tf	366.41	K	Cheméo Relay (1.0)
vc	0.323	m3/kmol	Cheméo Relay (1.0)

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C873621&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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