

Benzeneacetonitrile, 4-hydroxy-

Other names:	Acetonitrile, (p-hydroxyphenyl)- (4-Hydroxyphenyl)acetonitrile p-Hydroxybenzyl cyanide p-Hydroxyphenylacetonitrile 4-Hydroxybenzyl cyanide 4-Hydroxyphenylacetic acid nitrile
Inchi:	InChI=1S/C8H7NO/c9-6-5-7-1-3-8(10)4-2-7/h1-4,10H,5H2
InchiKey:	AYKYOOPFBCOXSL-UHFFFAOYSA-N
Formula:	C8H7NO
SMILES:	N#CCc1ccc(O)cc1
Mol. weight [g/mol]:	133.15
CAS:	14191-95-8

Physical Properties

Property code	Value	Unit	Source
gf	107.45	kJ/mol	Joback Method
hf	15.65	kJ/mol	Joback Method
hfus	17.81	kJ/mol	Joback Method
hvap	59.17	kJ/mol	Joback Method
ie	9.01 ± 0.05	eV	NIST Webbook
log10ws	-1.69		Crippen Method
logp	1.458		Crippen Method
mcvol	107.070	ml/mol	McGowan Method
pc	4266.28	kPa	Joback Method
tb	603.20	K	NIST Webbook
tc	834.93	K	Joback Method
tf	383.05	K	Joback Method
vc	0.367	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.07	J/mol×K	591.82	Joback Method
cpg	252.07	J/mol×K	632.34	Joback Method

cpg	260.36	J/mol×K	672.86	Joback Method
cpg	268.02	J/mol×K	713.37	Joback Method
cpg	275.14	J/mol×K	753.89	Joback Method
cpg	281.83	J/mol×K	794.41	Joback Method
cpg	288.17	J/mol×K	834.93	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	603.20	K	101.00	NIST Webbook

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=C14191958&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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