3-(4-Hydroxyphenyl)propionitrile

Other names:	«beta»-(4-Hydroxyphenyl)propionitrile
	Benzenepropanenitrile, 4-hydroxy-
	3-(p-Hydroxyphenyl)propiononitrile
Inchi:	InChI=1S/C9H9NO/c10-7-1-2-8-3-5-9(11)6-4-8/h3-6,11H,1-2H2
InchiKey:	KDMJGLYRWRHKJS-UHFFFAOYSA-N
Formula:	C9H9NO
SMILES:	N#CCCc1ccc(O)cc1
Mol. weight [g/mol]:	147.17
CAS:	17362-17-3

Physical Properties

Property code	Value	Unit	Source
gf	115.87	kJ/mol	Joback Method
hf	-4.99	kJ/mol	Joback Method
hfus	20.40	kJ/mol	Joback Method
hvap	61.40	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	1.848		Crippen Method
mcvol	121.160	ml/mol	McGowan Method
pc	3777.68	kPa	Joback Method
rinpol	1569.80		NIST Webbook
tb	614.70	K	Joback Method
tc	852.69	K	Joback Method
tf	394.32	K	Joback Method
vc	0.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.94	J/mol×K	614.70	Joback Method
cpg	297.96	J/mol×K	654.37	Joback Method
cpg	307.23	J/mol×K	694.03	Joback Method
cpg	315.86	J/mol×K	733.70	Joback Method
cpg	323.93	J/mol×K	773.36	Joback Method

cpg	331.55	J/mol×K	813.03	Joback Method
cpg	338.79	J/mol×K	852.69	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17362173&Units=SI

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume