3-Pyridinol

Other names:	3-Hydroxypyridine
	3-Oxopyridine
	3-Pyridol
	3-Pyridone
	pyridin-3-ol
	«beta»-Hydroxypyridine
	Â«betaÂ»-Hydroxypyridine
Inchi:	InChI=1S/C5H5NO/c7-5-2-1-3-6-4-5/h1-4,7H
InchiKey:	GRFNBEZIAWKNCO-UHFFFAOYSA-N
Formula:	C5H5NO
SMILES:	Oc1cccnc1
Mol. weight [g/mol]:	95.10
CAS:	109-00-2

Physical Properties

Property code	Value	Unit	Source
affp	929.50	kJ/mol	NIST Webbook
basg	897.70	kJ/mol	NIST Webbook
chs	-2550.10 ± 0.90	kJ/mol	NIST Webbook
hf	-43.70 ± 1.70	kJ/mol	NIST Webbook
hfs	-132.00 ± 1.10	kJ/mol	NIST Webbook
hsub	88.30 ± 1.30	kJ/mol	NIST Webbook
hsub	88.30 ± 1.30	kJ/mol	NIST Webbook
ie	9.50 ± 0.10	eV	NIST Webbook
ie	9.55 ± 0.02	eV	NIST Webbook
ie	9.55 ± 0.05	eV	NIST Webbook
ie	9.15 ± 0.03	eV	NIST Webbook
log10ws	-0.46		Aqueous Solubility Prediction Method
logp	0.787		Crippen Method
mcvol	73.400	ml/mol	McGowan Method
tf	400.40	K	Aqueous Solubility Prediction Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C109002&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point