

4-Pyridinol

Other names:	4-Hydroxypyridine 4-Pyridol 4-Pyridone pyridin-4-ol «gamma»-Hydroxypyridine Â«gammaÂ»-Hydroxypyridine
Inchi:	InChI=1S/C5H5NO/c7-5-1-3-6-4-2-5/h1-4H,(H,6,7)
InchiKey:	GCNTZFIIOFTKIY-UHFFFAOYSA-N
Formula:	C5H5NO
SMILES:	Oc1ccncc1
Mol. weight [g/mol]:	95.10
CAS:	626-64-2

Physical Properties

Property code	Value	Unit	Source
chs	-2533.20 ± 0.40	kJ/mol	NIST Webbook
chs	-2537.50 ± 1.10	kJ/mol	NIST Webbook
hf	-30.30 ± 5.30	kJ/mol	NIST Webbook
hf	-40.80 ± 2.10	kJ/mol	NIST Webbook
hfs	-144.60 ± 1.30	kJ/mol	NIST Webbook
hfs	-148.90 ± 0.80	kJ/mol	NIST Webbook
hsub	118.60 ± 5.20	kJ/mol	NIST Webbook
hsub	118.60 ± 5.20	kJ/mol	NIST Webbook
hsub	103.80 ± 1.70	kJ/mol	NIST Webbook
hsub	103.80 ± 1.70	kJ/mol	NIST Webbook
ie	9.70 ± 0.05	eV	NIST Webbook
ie	9.80 ± 0.03	eV	NIST Webbook
ie	9.60 ± 0.10	eV	NIST Webbook
ie	9.89 ± 0.02	eV	NIST Webbook
log10ws	1.02		Estimated Solubility Method
log10ws	1.02		Aqueous Solubility Prediction Method
logp	0.787		Crippen Method
mcvol	73.400	ml/mol	McGowan Method
rinpol	1154.00		NIST Webbook
rinpol	1154.00		NIST Webbook

tf	420.55	K	Aqueous Solubility Prediction Method
tf	421.15 ± 1.00	K	NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C626642&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

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
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point

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