4-PYRIDINOL

Other names:	4-Hydroxypyridine
	4-Pyridol
	4-Pyridone
	pyridin-4-ol
	«gamma»-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

Physical Properties

Property code	Value	Unit	Source
af	0.4718		Cheméo Relay (1.0)
chs	-2537.50 ± 1.10	kJ/mol	NIST Webbook
chs	-2533.20 ± 0.40	kJ/mol	NIST Webbook
gf	13.29	kJ/mol	Cheméo Relay (1.0, beta)
hf	-40.80 ± 2.10	kJ/mol	NIST Webbook
hf	-30.30 ± 5.30	kJ/mol	NIST Webbook
hfs	-148.90 ± 0.80	kJ/mol	NIST Webbook
hfs	-144.60 ± 1.30	kJ/mol	NIST Webbook
hsub	103.80 ± 1.70	kJ/mol	NIST Webbook
hsub	103.80 ± 1.70	kJ/mol	NIST Webbook
hsub	118.60 ± 5.20	kJ/mol	NIST Webbook
hsub	118.60 ± 5.20	kJ/mol	NIST Webbook
hvap	63.07	kJ/mol	Cheméo Relay (1.0)
ie	9.89 ± 0.02	eV	NIST Webbook
ie	9.80 ± 0.03	eV	NIST Webbook
ie	9.60 ± 0.10	eV	NIST Webbook
ie	9.70 ± 0.05	eV	NIST Webbook
log10ws	1.02		Aqueous Solubility Prediction Method
log10ws	1.02		Estimated Solubility Method
logp	0.787		Crippen Method
mcvol	73.400	ml/mol	McGowan Method
pc	6427.67	kPa	Cheméo Relay (1.0, beta)
rinpol	1154.00		NIST Webbook

rinpol	1154.00		NIST Webbook
tb	490.06	K	Cheméo Relay (1.0)
tc	732.65	K	Cheméo Relay (1.0)
tf	420.55	K	Aqueous Solubility Prediction Method
tf	421.15 ± 1.00	K	NIST Webbook
vc	0.236	m3/kmol	Cheméo Relay (1.0)

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C626642&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

af: Acentric Factor
chs: Standard solid enthalpy of combustion
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hsub: Enthalpy of sublimation 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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume