

2(1H)-Pyridinone

Other names:	«alpha»-Pyridone 2-Hydroxypyridine 2(1H)-Pyridone 2-Oxopyridine 2-Pyridinol 2-Pyridinone 2-Pyridone 2-Pyridol Pyridone-2 1-Hydroxy-2-pyridine 1H-Pyridin-2-one
Inchi:	InChI=1S/C5H5NO/c7-5-3-1-2-4-6-5/h1-4H,(H,6,7)
InchiKey:	UBQKCCHYAOITMY-UHFFFAOYSA-N
Formula:	C5H5NO
SMILES:	O=c1cccc[nH]1
Mol. weight [g/mol]:	95.10
CAS:	142-08-5

Physical Properties

Property code	Value	Unit	Source
hsub	86.60 ± 1.30	kJ/mol	NIST Webbook
ie	8.45 ± 0.00	eV	NIST Webbook
ie	8.62 ± 0.03	eV	NIST Webbook
ie	9.00 ± 0.10	eV	NIST Webbook
ie	8.45 ± 0.00	eV	NIST Webbook
log10ws	-0.11		Crippen Method
logp	-0.107		Crippen Method
mcvol	73.400	ml/mol	McGowan Method
rinpol	1094.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1095.00		NIST Webbook
rinpol	1094.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C142085&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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