

Ethanone, 1-(4-pyridinyl)-

Other names:	Ketone, methyl 4-pyridyl Methyl 4-pyridyl ketone 4-Acetylpyridine 4-Pyridyl methyl ketone Pyridine, 4-acetyl- «gamma»-Acetylpyridine 1-(4-Pyridinyl)ethanone
Inchi:	InChI=1S/C7H7NO/c1-6(9)7-2-4-8-5-3-7/h2-5H,1H3
InchiKey:	WMQUKDQWMMOHS-AUHFFFAOYSA-N
Formula:	C7H7NO
SMILES:	CC(=O)c1ccncc1
Mol. weight [g/mol]:	121.14
CAS:	1122-54-9

Physical Properties

Property code	Value	Unit	Source
affp	914.70	kJ/mol	NIST Webbook
basg	882.90	kJ/mol	NIST Webbook
hvap	66.50 ± 0.90	kJ/mol	NIST Webbook
ie	9.30	eV	NIST Webbook
ie	9.75	eV	NIST Webbook
log10ws	-1.90		Crippen Method
logp	1.284		Crippen Method
mcvol	97.280	ml/mol	McGowan Method
rinpol	1112.00		NIST Webbook
ripol	1801.00		NIST Webbook
ripol	1801.00		NIST Webbook
ripol	1800.00		NIST Webbook
tb	486.00 ± 1.00	K	NIST Webbook
tb	487.00	K	NIST Webbook
tb	485.20	K	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1122549&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature

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