

Ethanone, 1-(3-pyridinyl)-

Other names:	1-(3-Pyridinyl)ethanone 3-Acetopyridine 3-Pyridinyl methyl ketone 3-Pyridyl methyl ketone 3-acetylpyridine Ketone, methyl 3-pyridyl Methyl «beta»-pyridyl ketone NSC 761 methyl 3-pyridyl ketone pyridine, 3-acetyl- «beta»-Acetylpyridine
Inchi:	InChI=1S/C7H7NO/c1-6(9)7-3-2-4-8-5-7/h2-5H,1H3
InchiKey:	WEGYGNROSJDEIW-UHFFFAOYSA-N
Formula:	C7H7NO
SMILES:	CC(=O)c1cccnc1
Mol. weight [g/mol]:	121.14
CAS:	350-03-8

Physical Properties

Property code	Value	Unit	Source
affp	916.20	kJ/mol	NIST Webbook
basg	884.30	kJ/mol	NIST Webbook
hvap	66.10 ± 0.80	kJ/mol	NIST Webbook
ie	9.57	eV	NIST Webbook
ie	9.10	eV	NIST Webbook
log10ws	-1.90		Crippen Method
logp	1.284		Crippen Method
mcvol	97.280	ml/mol	McGowan Method
rinpol	1109.10		NIST Webbook
rinpol	1117.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1109.10		NIST Webbook
rinpol	1117.00		NIST Webbook
rinpol	1128.00		NIST Webbook
ripol	1833.00		NIST Webbook
ripol	1833.00		NIST Webbook
tb	493.00	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	379.00	K	1.60	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubilities of 3-acetylpyridine in supercritical carbon dioxide at several temperatures and pressures:	https://www.doi.org/10.1016/j.fluid.2013.06.036
3-acetylpyridine in supercritical carbon dioxide at several temperatures and pressures: Experimental and Modeling Fluid Phase Equilib. 354 (2013) 127-132.	https://www.doi.org/10.1016/j.fluid.2016.06.047
Crippen Method:	http://link.springer.com/article/10.1007/BF02311772
	http://webbook.nist.gov/cgi/cbook.cgi?ID=C350038&Units=SI
	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure

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