

Ethanone, 1-(2-pyridinyl)-

Other names:	Ketone, methyl 2-pyridyl Methyl 2-pyridyl ketone 2-Acetylpyridine 2-Pyridyl methyl ketone 2-Acetopyridine Acetyl pyridine 1-(2-pyridinyl)ethanone 2-Acetylpyridine
Inchi:	InChI=1S/C7H7NO/c1-6(9)7-4-2-3-5-8-7/h2-5H,1H3
InchiKey:	AJKVQEKCUCUMD-UHFFFAOYSA-N
Formula:	C7H7NO
SMILES:	CC(=O)c1ccccn1
Mol. weight [g/mol]:	121.14
CAS:	1122-62-9

Physical Properties

Property code	Value	Unit	Source
hvap	60.50 ± 0.30	kJ/mol	NIST Webbook
ie	8.90	eV	NIST Webbook
ie	9.35	eV	NIST Webbook
log10ws	-1.90		Crippen Method
logp	1.284		Crippen Method
mcvol	97.280	ml/mol	McGowan Method
rinpol	1005.00		NIST Webbook
rinpol	1026.00		NIST Webbook
rinpol	1050.00		NIST Webbook
rinpol	1026.00		NIST Webbook
rinpol	998.00		NIST Webbook
rinpol	1034.00		NIST Webbook
rinpol	1045.00		NIST Webbook
rinpol	1034.80		NIST Webbook
rinpol	1046.00		NIST Webbook
rinpol	1036.00		NIST Webbook
rinpol	1018.00		NIST Webbook
rinpol	1001.00		NIST Webbook
rinpol	1014.00		NIST Webbook
rinpol	991.00		NIST Webbook

rinpol	993.00	NIST Webbook
rinpol	998.00	NIST Webbook
rinpol	998.00	NIST Webbook
rinpol	1010.00	NIST Webbook
rinpol	1011.00	NIST Webbook
rinpol	1032.00	NIST Webbook
rinpol	1031.00	NIST Webbook
rinpol	1014.00	NIST Webbook
rinpol	999.00	NIST Webbook
rinpol	1032.00	NIST Webbook
rinpol	1050.00	NIST Webbook
rinpol	1057.00	NIST Webbook
rinpol	999.00	NIST Webbook
rinpol	1030.00	NIST Webbook
ripol	1586.00	NIST Webbook
ripol	1590.00	NIST Webbook
ripol	1608.00	NIST Webbook
ripol	1603.00	NIST Webbook
ripol	1603.00	NIST Webbook
ripol	1597.00	NIST Webbook
ripol	1602.00	NIST Webbook
ripol	1587.00	NIST Webbook
ripol	1615.00	NIST Webbook
ripol	1597.00	NIST Webbook
ripol	1599.00	NIST Webbook
ripol	1600.00	NIST Webbook
ripol	1567.00	NIST Webbook
ripol	1580.00	NIST Webbook
ripol	1587.00	NIST Webbook
ripol	1590.00	NIST Webbook
ripol	1552.00	NIST Webbook
ripol	1618.00	NIST Webbook
ripol	1599.00	NIST Webbook
ripol	1600.00	NIST Webbook
ripol	1560.00	NIST Webbook
ripol	1585.00	NIST Webbook
ripol	1585.00	NIST Webbook
ripol	1586.00	NIST Webbook
ripol	1587.00	NIST Webbook
ripol	1588.00	NIST Webbook
ripol	1602.00	NIST Webbook
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ripol	1587.00	NIST Webbook

ripol	1567.00		NIST Webbook
ripol	1618.00		NIST Webbook
ripol	1618.00		NIST Webbook
ripol	1608.00		NIST Webbook
ripol	1585.00		NIST Webbook
tb	465.00	K	NIST Webbook
tb	465.20	K	NIST Webbook
tb	461.70	K	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1122629&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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
ripol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

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