

# Ethanone, 1-(1H-pyrrol-2-yl)-

<b>Other names:</b>	1-(1H-pyrrol-2-yl)1-ethanone 1-(1H-pyrrol-2-yl)ethan-1-one 1-(1H-pyrrol-2-yl)ethanone 1-(1H-pyrrol-2-yl)ethanone (acetylpyrrole) 1-(1H-pyrrole-2-yl)-ethanone 1H-Pyrrole, 2-acetyl 2-Acetyl-1H-pyrrole 2-Pyrrolyl methyl ketone 2-acetylpyrrole Ethanone, 1-(1H-pyrrole-2-yl)- Ketone, methyl pyrrol-2-yl Methyl pyrrol-2-yl ketone Pyrrole, 2-acetyl Pyrrole-«alpha»-methyl ketone pyrrole, 2-acetyl-
<b>Inchi:</b>	InChI=1S/C6H7NO/c1-5(8)6-3-2-4-7-6/h2-4,7H,1H3
<b>InchiKey:</b>	IGJQUJNPMOYEJY-UHFFFAOYSA-N
<b>Formula:</b>	C6H7NO
<b>SMILES:</b>	CC(=O)c1ccc[nH]1
<b>Mol. weight [g/mol]:</b>	109.13
<b>CAS:</b>	1072-83-9

## Physical Properties

Property code	Value	Unit	Source
hfus	14.08	kJ/mol	Enthalpies of combustion and formation of 2-acetylpyrrole, 2-acetylfuran and 2-acetylthiophene
hsub	81.20 ± 1.00	kJ/mol	NIST Webbook
ie	8.72 ± 0.05	eV	NIST Webbook
log10ws	-1.35		Crippen Method
logp	0.735		Crippen Method
mcvol	87.490	ml/mol	McGowan Method
rinpol	1048.00		NIST Webbook
rinpol	1095.00		NIST Webbook
rinpol	1060.00		NIST Webbook
rinpol	1086.00		NIST Webbook

rinpol	1087.00	NIST Webbook
rinpol	1068.00	NIST Webbook
rinpol	1028.00	NIST Webbook
rinpol	1084.00	NIST Webbook
rinpol	1087.00	NIST Webbook
rinpol	1034.00	NIST Webbook
rinpol	1026.00	NIST Webbook
rinpol	1063.20	NIST Webbook
rinpol	1038.00	NIST Webbook
rinpol	1030.00	NIST Webbook
rinpol	1061.00	NIST Webbook
rinpol	1063.00	NIST Webbook
rinpol	1059.00	NIST Webbook
rinpol	1060.00	NIST Webbook
rinpol	1022.00	NIST Webbook
rinpol	1060.00	NIST Webbook
rinpol	1098.00	NIST Webbook
rinpol	1060.00	NIST Webbook
rinpol	1065.00	NIST Webbook
rinpol	1072.00	NIST Webbook
rinpol	1060.00	NIST Webbook
rinpol	1060.00	NIST Webbook
rinpol	1064.00	NIST Webbook
rinpol	1059.00	NIST Webbook
rinpol	1067.00	NIST Webbook
rinpol	1072.00	NIST Webbook
rinpol	1047.00	NIST Webbook
rinpol	1043.00	NIST Webbook
rinpol	1024.00	NIST Webbook
rinpol	1035.00	NIST Webbook
rinpol	1051.00	NIST Webbook
rinpol	1024.00	NIST Webbook
rinpol	1021.00	NIST Webbook
rinpol	1022.00	NIST Webbook
rinpol	1023.00	NIST Webbook
rinpol	1023.00	NIST Webbook
rinpol	1075.00	NIST Webbook
rinpol	1069.00	NIST Webbook
rinpol	1074.00	NIST Webbook
rinpol	1047.00	NIST Webbook
rinpol	1065.00	NIST Webbook
rinpol	1062.00	NIST Webbook
rinpol	1028.00	NIST Webbook
rinpol	1074.00	NIST Webbook

rinpol	1036.00	NIST Webbook
rinpol	1059.00	NIST Webbook
rinpol	1021.00	NIST Webbook
rinpol	1050.00	NIST Webbook
rinpol	1030.00	NIST Webbook
rinpol	1063.00	NIST Webbook
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rinpol	1026.00	NIST Webbook
rinpol	1084.00	NIST Webbook
rinpol	1063.00	NIST Webbook
rinpol	1064.00	NIST Webbook
rinpol	1050.00	NIST Webbook
rinpol	1063.20	NIST Webbook
rinpol	1058.00	NIST Webbook
ripol	1970.00	NIST Webbook
ripol	1959.00	NIST Webbook
ripol	1967.00	NIST Webbook
ripol	1952.00	NIST Webbook
ripol	1971.00	NIST Webbook
ripol	1975.00	NIST Webbook
ripol	1960.00	NIST Webbook
ripol	2002.00	NIST Webbook
ripol	1977.00	NIST Webbook
ripol	1977.00	NIST Webbook
ripol	1974.00	NIST Webbook
ripol	1933.00	NIST Webbook
ripol	1978.00	NIST Webbook
ripol	1977.00	NIST Webbook
ripol	2003.00	NIST Webbook
ripol	1970.00	NIST Webbook
ripol	1980.00	NIST Webbook
ripol	1980.00	NIST Webbook
ripol	1949.00	NIST Webbook
ripol	1983.00	NIST Webbook
ripol	2006.00	NIST Webbook
ripol	2003.00	NIST Webbook
ripol	2008.00	NIST Webbook
ripol	1967.00	NIST Webbook
ripol	2006.00	NIST Webbook
ripol	1960.00	NIST Webbook

ripol	1972.00		NIST Webbook
ripol	1943.00		NIST Webbook
ripol	1974.00		NIST Webbook
ripol	1984.00		NIST Webbook
ripol	1983.00		NIST Webbook
ripol	2006.00		NIST Webbook
ripol	1983.00		NIST Webbook
ripol	2006.00		NIST Webbook
ripol	2008.00		NIST Webbook
ripol	2003.00		NIST Webbook
ripol	1970.00		NIST Webbook
ripol	1970.00		NIST Webbook
ripol	1973.00		NIST Webbook
ripol	1925.00		NIST Webbook
ripol	1967.00		NIST Webbook
ripol	1957.00		NIST Webbook
ripol	1970.00		NIST Webbook
ripol	2020.00		NIST Webbook
ripol	1927.00		NIST Webbook
ripol	1983.00		NIST Webbook
ripol	1950.00		NIST Webbook
ripol	1969.00		NIST Webbook
ripol	1949.00		NIST Webbook
ripol	1950.00		NIST Webbook
ripol	1986.00		NIST Webbook
ripol	1935.00		NIST Webbook
ripol	1930.00		NIST Webbook
ripol	1930.00		NIST Webbook
ripol	1972.00		NIST Webbook
ripol	1966.00		NIST Webbook
ripol	1960.00		NIST Webbook
ripol	1959.00		NIST Webbook
tb	493.20	K	NIST Webbook
tb	493.00	K	NIST Webbook
tf	363.00 ± 3.00	K	NIST Webbook
tf	363.00	K	NIST Webbook

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	14.08	kJ/mol	363.00	NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1072839&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1072839&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Enthalpies of combustion and formation of 2-acetylpyrrole, 2-acetylthiophene, and 2-acetylpyrrole:</b>	<a href="https://www.doi.org/10.1016/j.tca.2009.04.012">https://www.doi.org/10.1016/j.tca.2009.04.012</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hfust:</b>	Enthalpy of fusion at a given temperature
<b>hsub:</b>	Enthalpy of sublimation at standard conditions
<b>hsubt:</b>	Enthalpy of sublimation at a given temperature
<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</b>	McGowan's characteristic volume
<b>rinpolar:</b>	Non-polar retention indices
<b>ripolar:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tf:</b>	Normal melting (fusion) point

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