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

Other names:	1-(1-Methylpyrrol-2-yl)ethanone
	2-Acetyl-1-methylpyrrole
	2-Acetyl-N-methylpyrrole
	N-Methyl-2-acetylpyrrole
	1H-Pyrrole, 1-methyl-2-acetyl
	1-Methyl-2-acetylpyrrole
	1-(1-methyl-1H-pyrrol-2-yl)ethanone
Inchi:	InChI=1S/C7H9NO/c1-6(9)7-4-3-5-8(7)2/h3-5H,1-2H3
InchiKey:	NZFLWVDXYUGFAV-UHFFFAOYSA-N
Formula:	C7H9NO
SMILES:	CC(=O)c1cccn1C
Mol. weight [g/mol]:	123.15
CAS:	932-16-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.42		Crippen Method
logp	1.228		Crippen Method
mcvol	101.580	ml/mol	McGowan Method
rinpol	1050.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1055.00		NIST Webbook
ripol	1653.00		NIST Webbook
ripol	1647.00		NIST Webbook
ripol	1645.00		NIST Webbook
ripol	1645.00		NIST Webbook
ripol	1647.00		NIST Webbook
ripol	1668.00		NIST Webbook
ripol	1609.00		NIST Webbook
ripol	1654.00		NIST Webbook
ripol	1657.00		NIST Webbook
ripol	1657.00		NIST Webbook
ripol	1660.00		NIST Webbook
ripol	1660.00		NIST Webbook
tb	474.20	K	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C932161&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

Latest version available from:

https://www.chemeo.com/cid/64-825-5/Ethanone-1-1-methyl-1H-pyrrol-2-yl.pdf

Generated by Cheméo on 2024-04-28 06:16:26.275062679 +0000 UTC m=+16574235.195640003.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.