

Ethanone, 1-(1H-pyrazol-4-yl)-

Other names:	Ketone, methyl pyrazol-4-yl 4-Acetylpyrazole 1-(1H-pyrazol-4-yl)ethanone
Inchi:	InChI=1S/C5H6N2O/c1-4(8)5-2-6-7-3-5/h2-3H,1H3,(H,6,7)
InchiKey:	SSGVCJCDGSZFI-UHFFFAOYSA-N
Formula:	C5H6N2O
SMILES:	CC(=O)c1cn[nH]c1
Mol. weight [g/mol]:	110.11
CAS:	25016-16-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.12		Crippen Method
logp	0.130		Crippen Method
mcvol	83.380	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25016164&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/66-151-1/Ethanone-1-1H-pyrazol-4-yl.pdf>

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