

# 3-hydroxy-2-pyranone

<b>Other names:</b>	3-hydroxy-2H-pyran-2-one 3-Hydroxy-2-pyrone
<b>Inchi:</b>	InChI=1S/C5H4O3/c6-4-2-1-3-8-5(4)7/h1-3,6H
<b>InchiKey:</b>	LIPRKYKMQPYPG-UHFFFAOYSA-N
<b>Formula:</b>	C5H4O3
<b>SMILES:</b>	O=c1occcc1O
<b>Mol. weight [g/mol]:</b>	112.08
<b>CAS:</b>	496-64-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.18		Crippen Method
logp	0.345		Crippen Method
mcvol	75.160	ml/mol	McGowan Method
ripol	989.00		NIST Webbook
ripol	959.00		NIST Webbook
ripol	959.00		NIST Webbook
ripol	989.00		NIST Webbook
ripol	959.00		NIST Webbook
ripol	959.00		NIST Webbook
ripol	1997.00		NIST Webbook
ripol	1997.00		NIST Webbook
ripol	1967.00		NIST Webbook
ripol	1965.00		NIST Webbook
ripol	1997.00		NIST Webbook
ripol	1965.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C496640&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C496640&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

# Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices

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