

# 2H-Pyran-2-one

<b>Other names:</b>	«alpha»-Pyrone Coumalin 2-Pyranone 2-Pyrone 2,4-Pentadienoic acid, 5-hydroxy-, «delta»-lactone 2H-Pyran, 2-oxo- Pyran-2-one
<b>Inchi:</b>	InChI=1S/C5H4O2/c6-5-3-1-2-4-7-5/h1-4H
<b>InchiKey:</b>	ZPSJGADGUYRKE-UHFFFAOYSA-N
<b>Formula:</b>	C5H4O2
<b>SMILES:</b>	O=c1cccc1
<b>Mol. weight [g/mol]:</b>	96.08
<b>CAS:</b>	504-31-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.63		Crippen Method
logp	0.640		Crippen Method
mcvol	69.290	ml/mol	McGowan Method
rinpol	983.00		NIST Webbook
rinpol	973.00		NIST Webbook
rinpol	973.00		NIST Webbook
rinpol	978.00		NIST Webbook
ripol	1505.00		NIST Webbook
tb	480.70	K	NIST Webbook

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	375.70	K	2.70	NIST Webbook

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C504314&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C504314&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>mcpvol:</b>	McGowan's characteristic volume
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure

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