

# 3-Cyclobutene-1,2-dione

<b>Other names:</b>	Diketocyclobutene
<b>Inchi:</b>	InChI=1S/C4H2O2/c5-3-1-2-4(3)6/h1-2H
<b>InchiKey:</b>	RGBVWCQARBEPW-UHFFFAOYSA-N
<b>Formula:</b>	C4H2O2
<b>SMILES:</b>	O=c1ccc1=O
<b>Mol. weight [g/mol]:</b>	82.06
<b>CAS:</b>	32936-74-6

## Physical Properties

Property code	Value	Unit	Source
ie	9.79	eV	NIST Webbook
log10ws	0.85		Crippen Method
logp	-0.717		Crippen Method
mcvol	55.200	ml/mol	McGowan Method

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C32936746&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C32936746&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>

## Legend

<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

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