

# Coumarin-3-carboxylic acid

<b>Other names:</b>	2-Oxobenzopyran-3-carboxylic acid 2-oxo-2H-1-benzopyran-3-carboxylic acid 2-oxo-2H-chromene-3-carboxylic acid 2H-1-Benzopyran-3-carboxylic acid, 2-oxo- 2H-1-benzopyran-2-one-3-carboxylic acid 3-carboxycoumarin Benzopyran-3-carboxylic acid, 2H-1-, 2-oxo G 1 Malonic acid, salicylidene-, «delta»-lactone
<b>Inchi:</b>	InChI=1S/C10H6O4/c11-9(12)7-5-6-3-1-2-4-8(6)14-10(7)13/h1-5H,(H,11,12)
<b>InchiKey:</b>	ACMLKANOOGIVEPB-UHFFFAOYSA-N
<b>Formula:</b>	C10H6O4
<b>SMILES:</b>	O=C(O)c1cc2ccccc2oc1=O
<b>Mol. weight [g/mol]:</b>	190.15
<b>CAS:</b>	531-81-7

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.49		Crippen Method
logp	1.491		Crippen Method
mcvol	127.720	ml/mol	McGowan Method

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Equilibrium partitioning of drug molecules between aqueous and amino acid solution:</b>	<a href="https://www.doi.org/10.1016/j.jct.2013.02.011">https://www.doi.org/10.1016/j.jct.2013.02.011</a>
<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=C531817&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C531817&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>

# Legend

**log10ws:** Log10 of Water solubility in mol/l

**logP:** Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume

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