

# Scopoletin

<b>Other names:</b>	7-Hydroxy-6-methoxy-2H-1-benzopyran-2-one Coumarin, 7-hydroxy-6-methoxy- «beta»-Methylesculetin Chrysotropic acid Gelseminic acid Murrayetin Scopoletine Scopoletol 6-Methoxy-7-hydroxycoumarin 6-Methylesculetin 7-Hydroxy-6-methoxycoumarin 2H-1-Benzopyran-2-one, 7-hydroxy-6-methoxy- Escopoletin Esculetin 6-methyl ether 6-O-Methylesculetin Buxuletin NSC 405647 7-Hydroxy-6-methoxy-2H-chromen-2-one
<b>Inchi:</b>	InChI=1S/C10H8O4/c1-13-9-4-6-2-3-10(12)14-8(6)5-7(9)11/h2-5,11H,1H3
<b>InchiKey:</b>	RODXRVNMMDRFIK-UHFFFAOYSA-N
<b>Formula:</b>	C10H8O4
<b>SMILES:</b>	<chem>COc1cc2ccc(=O)oc2cc1O</chem>
<b>Mol. weight [g/mol]:</b>	192.17
<b>CAS:</b>	92-61-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.10		Crippen Method
logp	1.507		Crippen Method
mccvol	132.020	ml/mol	McGowan Method
rinpol	1991.00		NIST Webbook
rinpol	1924.00		NIST Webbook
rinpol	1974.00		NIST Webbook
rinpol	1991.00		NIST Webbook
rinpol	1974.00		NIST Webbook

# 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=C92615&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C92615&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>

# 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>rinpola:</b>	Non-polar retention indices

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