

2H-1-Benzopyran-2-one, 7,8-dihydroxy-6-methoxy-

Other names:	Coumarin, 7,8-dihydroxy-6-methoxy Fraxetin 7,8-dihydroxy-6-methoxy-2-benzopyrone
Inchi:	InChI=1S/C10H8O5/c1-14-6-4-5-2-3-7(11)15-10(5)9(13)8(6)12/h2-4,12-13H,1H3
InchiKey:	HAVWRBANWNTQJX-UHFFFAOYSA-N
Formula:	C10H8O5
SMILES:	<chem>COc1cc2ccc(=O)oc2c(O)c1O</chem>
Mol. weight [g/mol]:	208.17
CAS:	574-84-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.65		Crippen Method
logp	1.213		Crippen Method
mcvol	137.890	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C574845&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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