

5,7-Dihydroxycoumarin

Inchi:	InChI=1S/C9H6O4/c10-5-3-7(11)6-1-2-9(12)13-8(6)4-5/h1-4,10-11H
InchiKey:	KIQQFVJHWNCGAU-UHFFFAOYSA-N
Formula:	C9H6O4
SMILES:	O=c1ccc2c(O)cc(O)cc2o1
Mol. weight [g/mol]:	178.14
CAS:	2732-18-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.53		Crippen Method
logp	1.204		Crippen Method
mcvol	117.930	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=C2732185&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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<https://www.chemeo.com/cid/30-739-8/5-7-Dihydroxycoumarin.pdf>

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