

7-Hydroxy-4,8-dimethylcoumarin

Inchi:	InChI=1S/C11H10O3/c1-6-5-10(13)14-11-7(2)9(12)4-3-8(6)11/h3-5,12H,1-2H3
InchiKey:	MVMMGVPSTRNMSV-UHFFFAOYSA-N
Formula:	C11H10O3
SMILES:	<chem>Cc1cc(=O)oc2c(C)c(O)ccc12</chem>
Mol. weight [g/mol]:	190.20
CAS:	4115-76-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.93		Crippen Method
logp	2.115		Crippen Method
mcvol	140.240	ml/mol	McGowan Method
rinpol	2026.00		NIST Webbook
rinpol	2013.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C4115768&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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