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: Cc1cc(=O)oc2c(C)c(O)ccc12
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