8-ACETYL-7-HYDROXY-4-METHYLCHROMEN-2-O

Other names: 8-Acetyl-7-hydroxy-4-methylcoumarin
4-Methyl-7-hydroxy-8-acetylcoumarin
Inchi: InChI=1S/C12H10O4/c1-6-5-10(15)16-12-8(6)3-4-9(14)11(12)7(2)13/h3-5,14H,1-2H3
InchiKey: WZOMQVFUPMLOGT-UHFFFAOYSA-N
Formula: C12H10O4
SMILES: CC(=O)c1c(O)ccc2c(C)cc(=O)oc12
Mol. weight [g/mol]: 218.21

Physical Properties

Property code	Value	Unit	Source
ie	8.12	eV	Cheméo Relay (1.0)
logp	2.010		Crippen Method
mcvol	155.900	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2555295&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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