

Coumarin, 8-acetyl-7-hydroxy-4-methyl-

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
CAS:	2555-29-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.12		Crippen Method
logp	2.010		Crippen Method
mcvol	155.900	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2555295&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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