

7-Acetoxy-4-methylcoumarin

Other names:	4-Methylumbelliferyl acetate «beta»-Methylumbelliferyl acetate 2H-1-Benzopyran-2-one, 7-(acetyloxy)-4-methyl- 7-(acetyloxy)-4-methyl-2-benzopyrone
Inchi:	InChI=1S/C12H10O4/c1-7-5-12(14)16-11-6-9(15-8(2)13)3-4-10(7)11/h3-6H,1-2H3
InchiKey:	HXVZGASCDAGAPS-UHFFFAOYSA-N
Formula:	C12H10O4
SMILES:	CC(=O)Oc1ccc2c(C)cc(=O)oc2c1
Mol. weight [g/mol]:	218.21
CAS:	2747-05-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.22		Crippen Method
logp	2.027		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=C2747059&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.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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