

5,7,8-trimethoxycoumarin

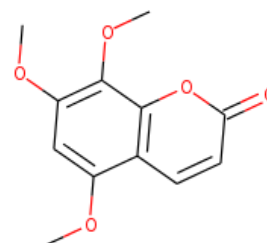
InChI: InChI=1S/C12H12O5/c1-14-8-6-9(15-2)12(16-3)11-7(8)4-5-10(13)17-11/h4-6H,1-3H3

InChI Key: MSFXSDYNQKVMTJ-UHFFFAOYSA-N

Formula: C12H12O5

SMILES: COc1cc(OC)c(OC)c2oc(=O)ccc12

Molecular Weight: 236.22



Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	1.82		Crippen Method

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H12O5/c1-14-8-6-9\(15-2\)12\(16-3\)11-7\(8\)4-5-10\(13\)17-11/h4-6H,1-3H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H12O5/c1-14-8-6-9(15-2)12(16-3)11-7(8)4-5-10(13)17-11/h4-6H,1-3H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

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<https://www.cheméo.com/cid/85-617-3/5%2C7%2C8-trimethoxycoumarin>

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