

3,4-(2'-METHYL-2'METHOXY-4'-PHENYL)-DIHYDR

Other names:	2H-Pyran-5-carboxylic acid, 3,4-dihydro-6-(9-hydroxyphenyl)-2-methoxy-2-methyl-4-phenyl-, «delta»-lactone 3,4-(2'-Methyl-2'-methoxy-4'-phenyl)dihydropyrano(2') coumann 3,4-(2'-Methyl-2'-methoxy-4'-phenyl)dihydropyranocoumarin 3,4-Dihydro-2-methoxy-2-methyl-4-phenyl-2H,5H-pyrano(3,2-c)(1)benzopyran-5-one 3,4-dihydro-2-methoxy-2-methyl-4-phenylpyrano[3,2-c]chromen-5-one Anticoagulans 63 Anticoagulant No. 63 BL 5 Compound 63 link Cumopyran Cumopyrin Cyclocoumarol Cyclocoumarol Methanopyranorin
Inchi:	InChI=1S/C20H18O4/c1-20(22-2)12-15(13-8-4-3-5-9-13)17-18(24-20)14-10-6-7-11-16(14)
InchiKey:	ZGFASEKBKWVCGP-UHFFFAOYSA-N
Formula:	C20H18O4
SMILES:	COC1(C)CC(c2ccccc2)c2c(c3ccccc3oc2=O)O1
Mol. weight [g/mol]:	322.36

Physical Properties

Property code	Value	Unit	Source
logp	4.070		Crippen Method
mcvol	238.300	ml/mol	McGowan Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C518207&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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