

2H,5H-Pyrano[3,2-c][1]benzopyran-5-one, 3,4-dihydro-2-methoxy-2-methyl-4-phenyl-

Other names:

Cyclocoumarol
Anticoagulans 63
BL 5
Compound 63 link
Cumopyran
Cumopyrin
Cyclocoumarol
3,4-Dihydro-2-methoxy-2-methyl-4-phenyl-2H,5H-pyrano(3,2-c)(1)benzopyran-5-one
Methanopyranorin
Anticoagulant No. 63
3,4-(2'-Methyl-2'-methoxy-4'-phenyl)dihydropyrano coumarin
2H-Pyran-5-carboxylic acid,
3,4-dihydro-6-(*o*-hydroxyphenyl)-2-methoxy-2-methyl-4-phenyl-, «delta»-lactone
3,4-(2'-Methyl-2'-methoxy-4'-phenyl)dihydropyrano(2') coumarin
3,4-dihydro-2-methoxy-2-methyl-4-phenylpyrano[3,2-c]chromen-5-one

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(14-10-6-7-11-16)
InchiKey: ZGFASEKKBKWC GP-UHFFFAOYSA-N
Formula: C20H18O4
SMILES: COC1(C)CC(c2ccccc2)c2c(c3ccccc3oc2=O)O1
Mol. weight [g/mol]: 322.35
CAS: 518-20-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.46		Crippen Method
logp	4.070		Crippen Method
mcvol	238.300	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
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C518207&Units=SI>

Legend

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

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