Dicumarol

Other names: 3,3'-Methylenebis(4-hydroxycoumarin)
2H-1-Benzopyran-2-one, 3,3'-methylenebis[4-hydroxy-
dicoumarin
Acadyl
Acavyl
Antitrombosin
Baracoumin
Bis(4-hydroxycoumarin-3-yl)methane
Bis-3,3'-(4-hydroxycoumarinyl)methane
Bishydroxycoumarin
BHC
Coumarin, 3,3'-methylenebis(4-hydroxy-
Cuma
Cumid
Di-(4-hydroxy-3-coumarinyl)methane
Di-4-hydroxy-3,3'-methylenedicoumarin
Dicoumal
Dicoumarol
Dicuman
Dicumaol R
Dicumarine
Dicumol
Dufalone
Kumoran
Melitoxin
Temparin
Trombosan
3,3'-Methyleen-bis(4-hydroxy-cumarine)
3,3'-Methylen-bis(4-hydroxy-cumarin)
3,3'-Methylene-bis(4-hydroxycoumarine)
3,3'-Methylenebis(4-hydroxy-1,2-benzopyrone)
3,3'-Metilen-bis(4-idrossi-cumarina)
Dikumarol
3,3'-Methylenebis(4-hydroxy-2H-1-benzopyran-2-one)
NC 034
NSC 17860
NSC 221570

Inchi: InChI=1S/C19H12O6/c20-16-10-5-1-3-7-14(10)24-18(22)12(16)9-13-17(21)11-6-2-4-8-15

InchiKey: DOBMPNYZJYQDGZ-UHFFFAOYSA-N

Formula: C19H12O6

SMILES: O=c1oc2ccccc2c(O)c1Cc1c(O)c2ccccc2oc1=O
Mol. weight [g/mol]: 336.30
CAS: 66-76-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.59		Crippen Method
logp	2.901		Crippen Method
mcvol	227.350	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=C66762&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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