

# Warfarin

## Other names:

(+/-)-Warfarin  
(Phenyl-1 acetyl-2 ethyl) 3-hydroxy-4 coumarin  
(RS)-Warfarin  
1-(4'-Hydroxy-3'-coumarinyl)-1-phenyl-3-butanone  
2H-1-Benzopyran-2-one, 4-hydroxy-3-(3-oxo-1-phenylbutyl)-  
3-(1'-Phenyl-2'-acetylethyl)-4-hydroxycoumarin  
3-(Acetylbenzyl)-4-hydroxycoumarin  
3-(Alpha-acetylbenzyl)-4-hydroxycoumarin  
3-(«alpha»-Acetylbenzyl)-4-hydroxycoumarin  
3-(«alpha»-Phenyl-«beta»-acetylaethyl)-4-hydroxycoumarin  
3-(«alpha»-Phenyl-«beta»-acetylethyl)-4-hydroxycoumarin  
3-(Â«alphaÂ»-Acetylbenzyl)-4-hydroxycoumarin  
3-(Â«alphaÂ»-Phenyl-Â«betaÂ»-acetylaethyl)-4-hydroxycoumarin  
3-(Â«alphaÂ»-Phenyl-Â«betaÂ»-acetylethyl)-4-hydroxycoumarin  
4-Hydroxy-3-(3-oxo-1-phenyl-butyl) coumarine  
4-Hydroxy-3-(3-oxo-1-phenyl-butyl)-cumarin  
4-Hydroxy-3-(3-oxo-1-phenylbutyl)-2H-1-benzopyran-2-one  
4-Hydroxy-3-(3-oxo-1-phenylbutyl)coumarin  
4-Idrossi-3-(3-oxo-1-fenil-butil)-cumarine  
Arab rat deth  
Athrombin-K  
Athrombine-K  
Brumolin  
Co-rax  
Compound 42  
Coumadin  
Coumafen  
Coumafene  
Coumaphen  
Coumarin, 3-(«alpha»-acetylbenzyl)-4-hydroxy-  
Coumarin, 3-(Â«alphaÂ»-acetylbenzyl)-4-hydroxy-  
Coumarins  
Coumefene  
Cov-R-tox  
D-Con  
DL-3-(a-Acetylbenzyl)-4-hydroxycoumarin  
Dethmor  
Dethnel  
Eastern states duocide  
Fasco fascrat powder

Frass-Ratron  
Kumader  
Kumadu  
Kumatox  
Kypfarin  
Latka 42  
Liqua-tox  
Maag Rattentod Cum  
Mar-Frin  
Martin's mar-frin  
Maveran  
Mouse pak  
Panwarfin  
Prothromadin  
RAX  
RCRA Waste number P001  
Rat & mice bait  
Rat-B-gon  
Rat-Gard  
Rat-Kill  
Rat-Mix  
Rat-Ola  
Rat-Trol  
Rat-a-way  
Rat-o-cide No. 2  
Ratorex  
Ratox  
Ratoxin  
Ratron  
Ratron G  
Rats-no-more  
Ratten-Koederrohr  
Ratten-Koederrohr (German)  
Rattenstreupulver Neu Schacht  
Rattenstreupulver Neu Schacht (German)  
Rattentraenke  
Rattentraenke (German)  
Rattunal  
Rcr grey squirrel killer concentrate  
Ro-Deth  
Rodafarin  
Rodex  
Rodex blox

Rosex  
 Rough & ready mouse mix  
 Sakarat  
 Sewarin  
 Solfarin  
 Sorexa plus  
 Spray-trol brand roden-trol  
 Temus W  
 Tox-hid  
 Twin light rat away  
 Vampirinip II  
 Vampirinip III  
 W.A.R.F. 42  
 WARF compound 42  
 Waran  
 Warfarat  
 Warfarin Q  
 Warfarin plus  
 Warfarine  
 Warficide  
 Zoocoumarin

**Inchi:** InChI=1S/C19H16O4/c1-12(20)11-15(13-7-3-2-4-8-13)17-18(21)14-9-5-6-10-16(14)23-19  
**InchiKey:** PJVWKTQMONHTI-UHFFFAOYSA-N  
**Formula:** C19H16O4  
**SMILES:** CC(=O)CC(c1cccc1)c1c(O)c2cccc2oc1=O  
**Mol. weight [g/mol]:** 308.33  
**CAS:** 81-81-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.14		Aqueous Solubility Prediction Method
log10ws	-3.89		Estimated Solubility Method
logp	3.610		Crippen Method
mcvol	230.770	ml/mol	McGowan Method
rinpol	2625.00		NIST Webbook
rinpol	2625.00		NIST Webbook
rinpol	2625.00		NIST Webbook
tf	433.95	K	Aqueous Solubility Prediction Method

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# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Aqueous Solubility Prediction Method:</b>	<a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa</a>
<b>Estimated Solubility Method:</b>	<a href="http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt">http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C81812&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C81812&amp;Units=SI</a>

# Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rinpol:</b>	Non-polar retention indices
<b>tf:</b>	Normal melting (fusion) point

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