

Coumachlor

Other names:

(.+/-)-Coumachlor
2H-1-Benzopyran-2-one, 3-[1-(4-chlorophenyl)-3-oxobutyl]-4-hydroxy-
3-(1-(4-Chloorfenyl)-3-oxo-butyl)-4-hydroxy-cumarine
3-(1-(4-Chlor-phenyl)-3-oxo-butyl)-4-hydroxy-cumarin
3-(1-(4-Chlorophenyl)-3-oxo-butyl)-4-hydroxy-coumarine
3-(1-(4-Cloro-fenil)-3-oxo-butil)-4-idrossicumarina
3-(1-Acetyl-2-(p-chlorophenyl)ethyl)-4-hydroxycoumarin
3-(«alpha»-(p-Chlorphenyl)-«beta»-acetylaethyl)-4-hydroxycoumarin
3-(«alpha»-Acetonyl-4-chlorobenzyl)-4-hydroxycoumarin
3-(«alpha»-Acetonyl-p-chlorobenzyl)-4-hydroxycoumarin
3-(«alpha»-p-Chlorophenyl-«beta»-acetylethyl)-4-hydroxycoumarin
3-(«alpha»-(p-Chlorphenyl)-«beta»-acetylaethyl)-4-hydroxycoumarin
3-(«alpha»-Acetonyl-4-chlorobenzyl)-4-hydroxycoumarin
3-(«alpha»-Acetonyl-p-chlorobenzyl)-4-hydroxycoumarin
3-(«alpha»-p-Chlorophenyl-«beta»-acetylethyl)-4-hydroxycoumarin
4-Hydroxy-3-[3-oxo-1-(4-chlorophenyl)butyl]coumarin
Coumachlore
Coumarin, 3-(«alpha»-acetonyl-p-chlorobenzyl)-4-hydroxy-
Coumarin, 3-(«alpha»-acetonyl-p-chlorobenzyl)-4-hydroxy-
Cumachloor
Cumachlor
Experimental Rodenticide 332
G-23133
Geigy Rodenticide Exp. 332
Kumachlor
Ratilan
Tomorin
dl-3-(«alpha»-Acetonyl-4-chlorobenzyl)-4-hydroxycoumarin
dl-3-(«alpha»-Acetonyl-4-chlorobenzyl)-4-hydroxycoumarin

Inchi: InChI=1S/C19H15ClO4/c1-11(21)10-15(12-6-8-13(20)9-7-12)17-18(22)14-4-2-3-5-16(14)

InchiKey: DEKWZWCFFHUABHE-UHFFFAOYSA-N

Formula: C19H15ClO4

SMILES: CC(=O)CC(c1ccc(Cl)cc1)c1c(O)c2ccccc2oc1=O

Mol. weight [g/mol]: 342.77

CAS: 81-82-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.84		Aqueous Solubility Prediction Method
log10ws	-5.84		Estimated Solubility Method
logp	4.263		Crippen Method
mcvol	243.010	ml/mol	McGowan Method

Sources

Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C81823&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

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

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