# 2H-1-Benzopyran-2-one, 3-[1-(4-chlorophenyl)-3-oxobutyl]-4-hydroxy-

**Other names:** (.+/-.)-Coumachlor
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-hydroxycumarin
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
Coumachlor
Coumachlore
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

**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:** DEKWZWCFHUABHE-UHFFFAOYSA-N

**Formula:** C19H15ClO4

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

**Mol. weight [g/mol]:** 342.78

# 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 |

| | | | |
|---|---|---|---|
| tf | 425.90 | K | Cheméo Relay (1.0) |

# Sources

**Cheméo Relay (1.0, beta):**

**Aqueous Solubility Prediction Method:** http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

**Estimated Solubility Method:** http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C81823&Units=SI

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Cheméo Relay (1.0):**

# Legend

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume

**tf:** Normal melting (fusion) point