

Acenocoumarol

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| Other names: | 2H-1-Benzopyran-2-one, 4-hydroxy-3-[1-(4-nitrophenyl)-3-oxobutyl]- Coumarin, 3-(«alpha»-acetyl-p-nitrobenzyl)-4-hydroxy- Acenocoumarin Acenocumarol Acenokumarin 3-(«alpha»-Acetyl-p-nitrobenzyl)-4-hydroxy-coumarin 3-(«alpha»-Acetyl-4-nitrobenzyl)-4-hydroxycoumarin Ascumar G-23350 4-Hydroxy-3-(1-(4-nitrophenyl)-3-oxobutyl)-2H-1-benzopyran-2-one Nicoumalone 3-(«alpha»-(p-Nitrophenol)-«beta»-acetylethyl)-4-hydroxycoumarin Nitrophenylacetylethyl-4-hydroxycoumarine 3-(«alpha»-p-Nitrophenyl-«beta»-acetylethyl)-4-hydroxycoumarin 3-(«alpha»-(4-Nitrophenyl)-«beta»-acetylethyl)-4-hydroxycoumarin Nitrovarfarian Nitrowarfarin Sincoumar Sinkumar Sinthrom Sinthrome Sintrom Sintroma Syncoumar Syncumar Syntrom Zotil 3-(«alpha»-Acetyl-p-nitrophenyl)-4-hydroxycoumarin Minisintrom 3-(alpha-Acetyl-4-nitrobenzyl)-4-hydroxycoumarin Acitrom Trombostop |
| Inchi: | InChI=1S/C19H15NO6/c1-11(21)10-15(12-6-8-13(9-7-12)20(24)25)17-18(22)14-4-2-3-5- |
| InchiKey: | VABCILAOYCMVPS-UHFFFAOYSA-N |
| Formula: | C19H15NO6 |
| SMILES: | CC(=O)CC(c1ccc([N+](=O)[O-])cc1)c1c(O)c2ccccc2oc1=O |
| Mol. weight [g/mol]: | 353.33 |
| CAS: | 152-72-7 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -9.23 | | Crippen Method |
| logp | 3.518 | | Crippen Method |
| mcvol | 248.190 | ml/mol | McGowan Method |
| rinsol | 1779.00 | | NIST Webbook |
| rinsol | 1779.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C152727&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.cheméo.com/doc/models/crippen_log10ws |

Legend

| | |
|-----------------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| rinsol: | Non-polar retention indices |

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