ACENOCOUMAROL

Other names:	2H-1-Benzopyran-2-one, 4-hydroxy-3-[1-(4-nitrophenyl)-3-oxobutyl]-
	Coumarin, 3-(«alpha»-acetonyl-p-nitrobenzyl)-4-hydroxy-
	Acenocoumarin
	Acenocumarol
	Acenokumarin
	3-(«alpha»-Acetonyl-p-nitrobenzyl)-4-hydroxy-coumarin
	3-(«alpha»-Acetonyl-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»-Acetonyl-p-nitrophenyl)-4-hydroxycoumarin
	Minisintrom
	3-(alpha-Acetonyl-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

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.22		Cheméo Relay (1.0)
logp	3.518		Crippen Method
mcvol	248.190	ml/mol	McGowan Method
rinpol	1779.00		NIST Webbook
rinpol	1779.00		NIST Webbook
tf	440.41	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C152727&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

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