Phenprocoumon

Other names:	2H-1-Benzopyran-2-one, 4-hydroxy-3-(1-phenylpropyl)-
	Coumarin, 3-(«alpha»-ethylbenzyl)-4-hydroxy-
	Falithrom
	Fencumar
	Liquamar
	Marcoumar
	Marcumar
	Phenprocoumarol
	Phenprocoumarole
	3-(1'-Phenyl-propyl)-4-oxycoumarin
	Ro 1-4849
	3-(«alpha»-Ethylbenzyl)-4-hydroxycoumarin
	Phenprocumone
	3-(1-Phenylpropyl)-4-hydroxycoumarin
	4-Hydroxy-3-(1-phenylpropyl)-2H-1-benzopyran-2-one
Inchi:	InChI=1S/C18H16O3/c1-2-13(12-8-4-3-5-9-12)16-17(19)14-10-6-7-11-15(14)21-18(16)20
InchiKey:	DQDAYGNAKTZFIW-UHFFFAOYSA-N
Formula:	C18H16O3
SMILES:	CCC(c1ccccc1)c1c(O)c2ccccc2oc1=O
Mol. weight [g/mol]:	280.32
CAS:	435-97-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.88		Crippen Method
logp	4.040		Crippen Method
mcvol	215.110	ml/mol	McGowan Method
tf	456.00 ± 1.00	K	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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