4'-Methoxy-5,7-dihydroxy isoflavone

Other names:	4H-1-Benzopyran-4-one, 5,7-dihydroxy-3-(4-methoxyphenyl)-
	Biochanin
	Biochanin A
	Biochanine A
	Genistein 4-methyl ether
	Isoflavone, 5,7-dihydroxy-4'-methoxy-
	4'-Methylgenistein
	5,7-Dihydroxy-4'-methoxyisoflavone
	5,7-dihydroxy-3-p-methoxyphenyl-4H-chromen-4-one
	5,7-Dihydroxy-3-(4-methoxyphenyl)-4H-chromen-4-one
Inchi:	InChI=1S/C16H12O5/c1-20-11-4-2-9(3-5-11)12-8-21-14-7-10(17)6-13(18)15(14)16(12)19
InchiKey:	WUADCCWRTIWANL-UHFFFAOYSA-N
Formula:	C16H12O5
SMILES:	COc1ccc(-c2coc3cc(O)cc(O)c3c2=O)cc1
Mol. weight [g/mol]:	284.26
CAS:	491-80-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.25		Crippen Method
logp	2.880		Crippen Method
mcvol	198.670	ml/mol	McGowan Method
rinpol	2927.10		NIST Webbook
rinpol	2927.10		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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C491805&Units=SI

Legend

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