Ficusin

Other names:	2-Propenoic acid, 3-(6-hydroxy-5-benzofuranyl)-, «delta»-lactone
	2-Propenoic acid, 3-(6-hydroxy-5-benzofuranyl)-, Â«deltaÂ»-lactone
	5-Benzofuranacrylic acid, 6-hydroxy-, «delta»-lactone
	5-Benzofuranacrylic acid, 6-hydroxy-, Â«deltaÂ»-lactone
	6,7-Furanocoumarin
	7H-Furo[3,2-g][1]benzopyran-7-one
	Furo(2',3',7,6)coumarin
	Furo(4',5',6,7)coumarin
	Furo[2',3':7,6]coumarin
	Furo[2'.3':7.6]coumarin
	Furo[4',5':6,7]coumarin
	Furocoumarin
	NSC 404562
	Psoralen
	Psoralene
	Psorline-P
	furo[3,2-g]chromen-7-one
Inchi:	InChI=1S/C11H6O3/c12-11-2-1-7-5-8-3-4-13-9(8)6-10(7)14-11/h1-6H
InchiKey:	ZCCUUQDIBDJBTK-UHFFFAOYSA-N
Formula:	C11H6O3
SMILES:	O=c1ccc2cc3ccoc3cc2o1
Mol. weight [g/mol]:	186.16
CAS:	66-97-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.74		Aqueous Solubility Prediction Method
logp	2.539		Crippen Method
mcvol	125.080	ml/mol	McGowan Method
rinpol	1830.00		NIST Webbook
rinpol	1828.00		NIST Webbook
rinpol	1805.00		NIST Webbook
rinpol	1805.00		NIST Webbook
rinpol	1847.30		NIST Webbook
rinpol	1842.00		NIST Webbook

tf	436.65	K	Aqueous Solubility Prediction Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C66977&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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